



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:33 PM UTC

PDB ID : 1HXM / pdb_00001hxm
Title : Crystal Structure of a Human Vgamma9/Vdelta2 T Cell Receptor
Authors : Allison, T.J.; Winter, C.C.; Fournie, J.J.; Bonneville, M.; Garboczi, D.N.
Deposited on : 2001-01-16
Resolution : 3.12 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

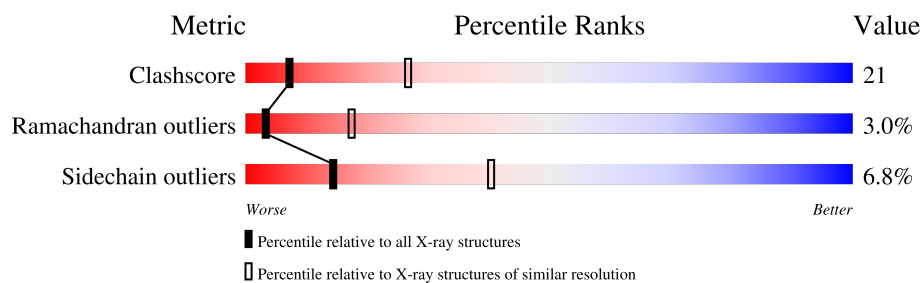
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)

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	229	57% 30% • 10%
1	C	229	54% 32% • 10%
1	E	229	51% 34% 5% 10%
1	G	229	54% 30% 6% 10%
2	B	242	55% 33% 7% 5%
2	D	242	57% 31% 7% 5%
2	F	242	56% 32% 7% 5%
2	H	242	57% 27% 10% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13820 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 GAMMA-DELTA T-CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1611	1022	270	310	9			
1	C	206	Total	C	N	O	S	0	0	0
			1611	1022	270	310	9			
1	E	206	Total	C	N	O	S	0	0	0
			1611	1022	270	310	9			
1	G	206	Total	C	N	O	S	0	0	0
			1611	1022	270	310	9			

- Molecule 2 is a protein called GAMMA-DELTA T-CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	230	Total	C	N	O	S	0	0	0
			1828	1167	304	351	6			
2	D	230	Total	C	N	O	S	0	0	0
			1828	1167	304	351	6			
2	F	230	Total	C	N	O	S	0	0	0
			1828	1167	304	351	6			
2	H	230	Total	C	N	O	S	0	0	0
			1828	1167	304	351	6			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

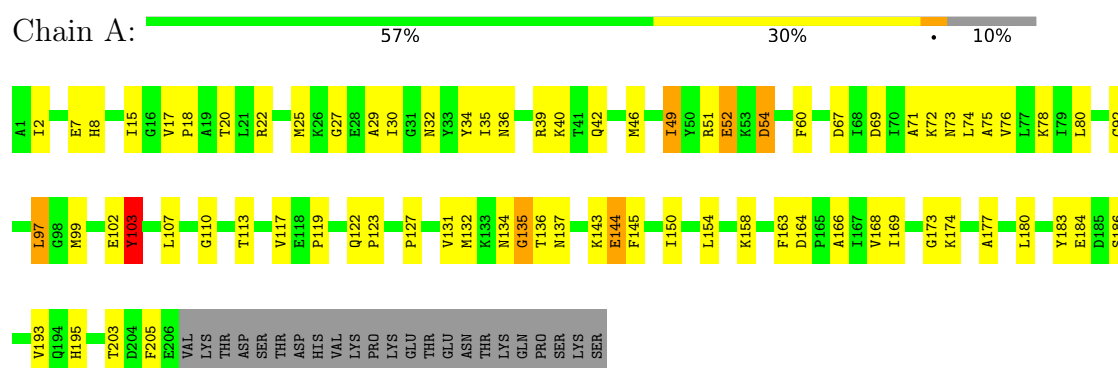
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	12	Total	O	0	0
			12	12		
4	C	2	Total	O	0	0
			2	2		
4	D	2	Total	O	0	0
			2	2		
4	E	8	Total	O	0	0
			8	8		
4	F	8	Total	O	0	0
			8	8		
4	G	7	Total	O	0	0
			7	7		
4	H	10	Total	O	0	0
			10	10		

3 Residue-property plots

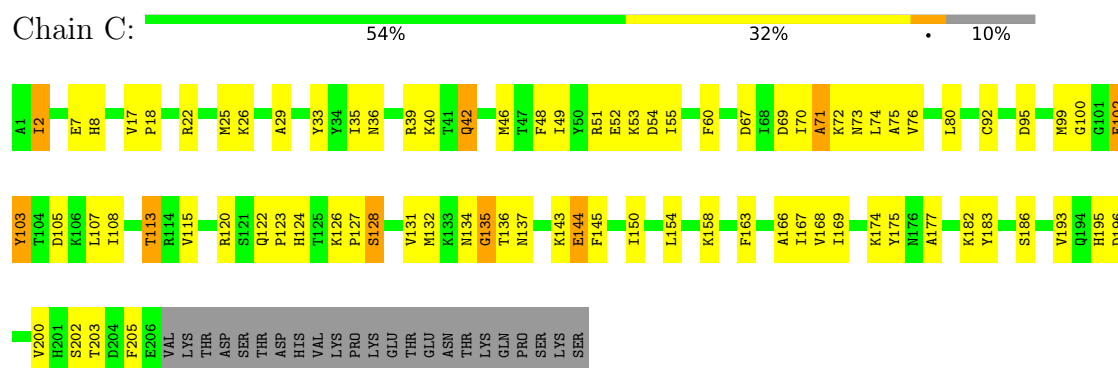
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

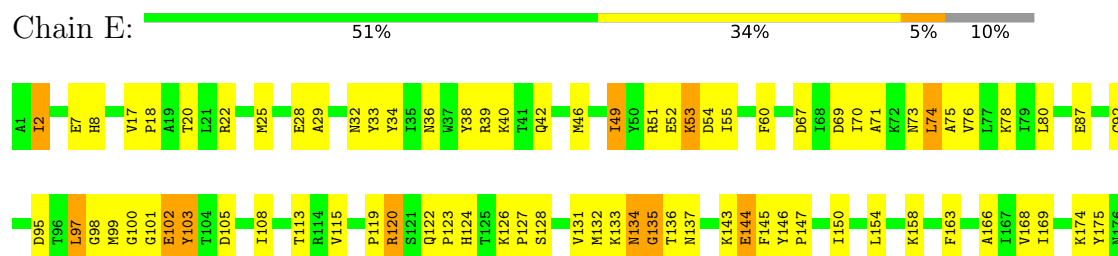
• Molecule 1: GAMMA-DELTA T-CELL RECEPTOR



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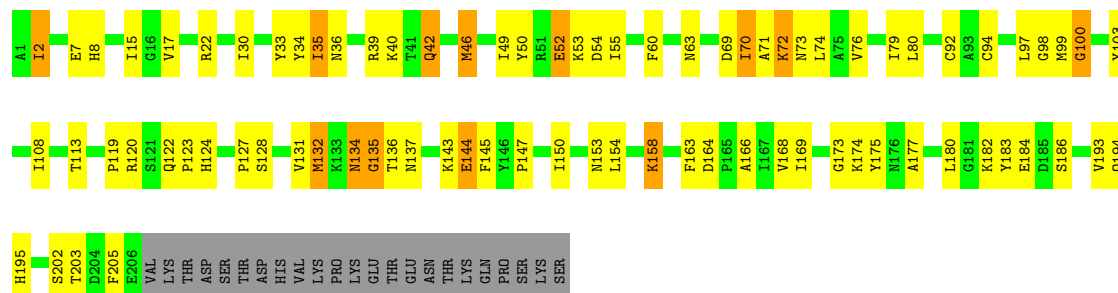


• Molecule 1: GAMMA-DELTA T-CELL RECEPTOR

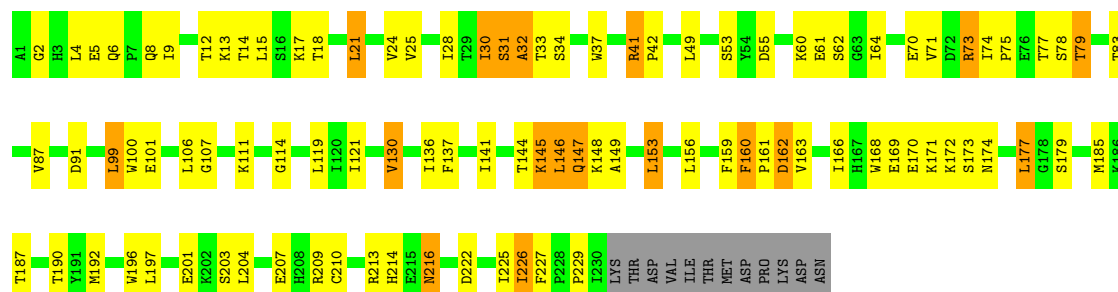




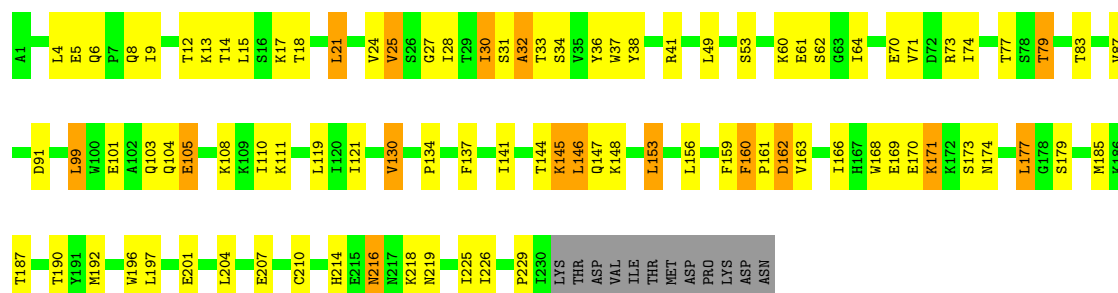
• Molecule 1: GAMMA-DELTA T-CELL RECEPTOR



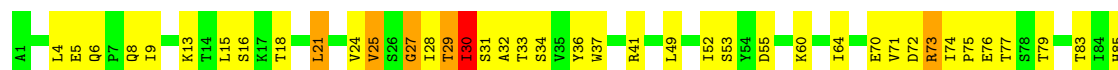
• Molecule 2: GAMMA-DELTA T-CELL RECEPTOR

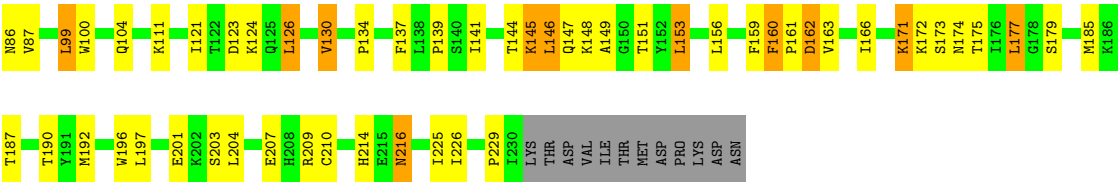


• Molecule 2: GAMMA-DELTA T-CELL RECEPTOR

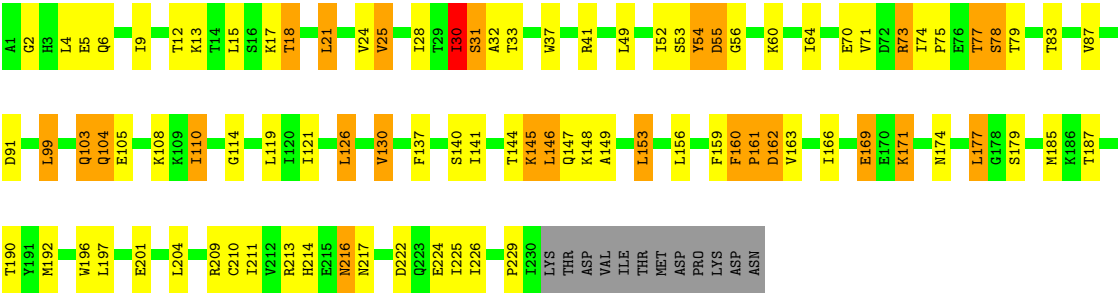


• Molecule 2: GAMMA-DELTA T-CELL RECEPTOR





• Molecule 2: GAMMA-DELTA T-CELL RECEPTOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.05Å 151.74Å 97.87Å 90.00° 99.48° 90.00°	Depositor
Resolution (Å)	30.77 – 3.12	Depositor
% Data completeness (in resolution range)	99.0 (30.77-3.12)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.219 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13820	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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: SO4

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	0.50	0/1646	0.95	4/2228 (0.2%)
1	C	0.47	0/1646	0.95	6/2228 (0.3%)
1	E	0.53	0/1646	0.97	6/2228 (0.3%)
1	G	0.56	1/1646 (0.1%)	0.99	5/2228 (0.2%)
2	B	0.56	0/1867	1.03	10/2529 (0.4%)
2	D	0.52	0/1867	1.02	11/2529 (0.4%)
2	F	0.54	0/1867	1.06	12/2529 (0.5%)
2	H	0.52	0/1867	1.04	12/2529 (0.5%)
All	All	0.53	1/14052 (0.0%)	1.00	66/19028 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	46	MET	SD-CE	-5.51	1.65	1.79

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	147	GLN	N-CA-C	-9.28	102.54	112.93
2	B	147	GLN	N-CA-C	-9.11	102.73	112.93
2	D	147	GLN	N-CA-C	-8.98	102.87	112.93
2	F	147	GLN	N-CA-C	-8.71	103.18	112.93
2	D	160	PHE	N-CA-C	7.62	126.66	109.81
2	F	160	PHE	N-CA-C	7.42	126.22	109.81
2	H	160	PHE	N-CA-C	7.38	126.11	109.81
2	B	160	PHE	N-CA-C	7.36	126.06	109.81
2	H	177	LEU	N-CA-C	7.24	114.72	108.78
2	F	74	ILE	CA-C-N	7.23	127.23	119.28
2	F	74	ILE	C-N-CA	7.23	127.23	119.28
2	D	177	LEU	N-CA-C	6.95	114.48	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	177	LEU	N-CA-C	6.89	114.43	108.78
2	F	177	LEU	N-CA-C	6.81	114.36	108.78
1	E	49	ILE	CB-CA-C	-6.64	106.07	111.71
1	C	54	ASP	N-CA-C	6.61	120.62	111.90
2	F	6	GLN	CA-C-N	6.57	126.81	119.32
2	F	6	GLN	C-N-CA	6.57	126.81	119.32
1	G	54	ASP	N-CA-C	6.50	120.48	111.90
2	H	73	ARG	N-CA-C	6.24	119.01	107.60
2	H	6	GLN	CA-C-N	6.05	126.22	119.32
2	H	6	GLN	C-N-CA	6.05	126.22	119.32
1	A	17	VAL	N-CA-C	5.94	113.43	107.55
2	H	77	THR	N-CA-C	-5.81	106.09	112.72
1	A	49	ILE	CB-CA-C	-5.71	106.86	111.71
1	E	17	VAL	N-CA-C	5.62	113.12	107.55
1	G	17	VAL	N-CA-C	5.62	113.11	107.55
2	B	6	GLN	CA-C-N	5.58	125.68	119.32
2	B	6	GLN	C-N-CA	5.58	125.68	119.32
1	C	17	VAL	N-CA-C	5.58	113.07	107.55
2	H	114	GLY	N-CA-C	-5.57	105.25	112.10
2	H	177	LEU	CB-CA-C	-5.53	109.11	117.07
2	D	216	ASN	N-CA-C	5.46	119.25	112.59
2	B	114	GLY	N-CA-C	-5.43	105.42	112.10
2	D	74	ILE	CA-C-N	5.38	125.45	119.32
2	D	74	ILE	C-N-CA	5.38	125.45	119.32
1	E	124	HIS	N-CA-C	5.35	117.23	110.33
2	D	177	LEU	CB-CA-C	-5.35	109.37	117.07
1	C	143	LYS	N-CA-C	5.32	118.16	109.59
2	B	203	SER	N-CA-C	5.32	119.26	112.87
2	B	177	LEU	CB-CA-C	-5.32	109.41	117.07
2	H	216	ASN	N-CA-C	5.30	119.06	112.59
2	F	27	GLY	N-CA-C	-5.30	108.32	115.36
2	B	216	ASN	N-CA-C	5.29	119.28	112.41
1	E	128	SER	N-CA-C	-5.27	101.69	110.17
2	F	203	SER	N-CA-C	5.24	119.16	112.87
1	E	133	LYS	N-CA-C	5.24	116.62	109.18
1	C	128	SER	N-CA-C	-5.21	101.79	110.17
2	F	216	ASN	N-CA-C	5.19	118.93	112.59
1	E	108	ILE	N-CA-C	-5.18	100.86	108.11
1	G	128	SER	N-CA-C	-5.17	101.72	109.95
1	C	202	SER	N-CA-C	-5.17	105.82	111.82
1	A	54	ASP	N-CA-C	5.14	121.75	110.80
2	H	169	GLU	N-CA-C	5.14	115.17	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	226	ILE	N-CA-C	5.14	116.09	108.23
2	F	177	LEU	CB-CA-C	-5.13	109.69	117.07
1	A	110	GLY	N-CA-C	-5.12	102.78	112.10
1	G	202	SER	N-CA-C	-5.12	105.89	111.82
2	B	226	ILE	N-CA-C	5.10	116.03	108.23
2	D	105	GLU	N-CA-C	5.09	118.01	110.48
2	F	226	ILE	N-CA-C	5.08	116.01	108.23
1	G	79	ILE	N-CA-C	-5.08	100.57	107.99
2	D	6	GLN	CA-C-N	5.04	125.07	119.32
2	D	6	GLN	C-N-CA	5.04	125.07	119.32
1	C	71	ALA	N-CA-C	-5.03	105.93	111.71
2	H	226	ILE	N-CA-C	5.01	115.89	108.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1611	0	1597	60	0
1	C	1611	0	1597	57	0
1	E	1611	0	1597	72	0
1	G	1611	0	1597	64	0
2	B	1828	0	1848	105	0
2	D	1828	0	1848	80	0
2	F	1828	0	1848	86	0
2	H	1828	0	1848	86	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
4	A	5	0	0	0	0
4	B	12	0	0	3	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	8	0	0	2	0
4	F	8	0	0	1	0
4	G	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	10	0	0	0	0
All	All	13820	0	13780	570	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 21.

All (570) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:153:LEU:HD12	2:F:196:TRP:HB3	1.42	1.02
1:C:127:PRO:HB3	1:C:145:PHE:HB3	1.38	1.02
1:A:127:PRO:HB3	1:A:145:PHE:HB3	1.39	1.00
1:E:127:PRO:HB3	1:E:145:PHE:HB3	1.38	0.99
2:D:153:LEU:HD12	2:D:196:TRP:HB3	1.40	0.99
2:H:153:LEU:HD12	2:H:196:TRP:HB3	1.45	0.99
1:A:36:ASN:HD21	1:A:51:ARG:HH11	1.04	0.98
1:G:127:PRO:HB3	1:G:145:PHE:HB3	1.41	0.98
2:B:153:LEU:HD12	2:B:196:TRP:HB3	1.47	0.97
2:B:30:ILE:HD12	2:B:30:ILE:H	1.28	0.96
2:H:171:LYS:HA	2:H:209:ARG:HH22	1.31	0.95
1:C:36:ASN:HD21	1:C:51:ARG:HH11	1.11	0.94
2:H:130:VAL:HG13	2:H:160:PHE:H	1.34	0.93
2:D:130:VAL:HG13	2:D:160:PHE:H	1.34	0.92
2:F:130:VAL:HG13	2:F:160:PHE:H	1.33	0.92
2:F:171:LYS:HG2	2:F:207:GLU:HB3	1.52	0.90
1:C:29:ALA:HA	1:C:73:ASN:HD21	1.37	0.90
2:B:130:VAL:HG13	2:B:160:PHE:H	1.38	0.89
2:F:171:LYS:HA	2:F:209:ARG:HH12	1.36	0.89
1:C:39:ARG:HB3	1:C:49:ILE:HD11	1.56	0.88
2:D:171:LYS:HB2	2:D:207:GLU:HB3	1.53	0.87
1:A:122:GLN:HB2	1:A:123:PRO:HD2	1.59	0.84
1:A:39:ARG:HB3	1:A:49:ILE:HD11	1.59	0.82
1:A:20:THR:HG22	1:A:78:LYS:HG3	1.60	0.81
1:A:22:ARG:HG2	1:A:76:VAL:HG12	1.63	0.80
1:E:39:ARG:HB3	1:E:49:ILE:HD11	1.64	0.79
1:G:30:ILE:HD11	1:G:35:ILE:HD11	1.65	0.78
1:E:22:ARG:HG2	1:E:76:VAL:HG12	1.65	0.78
1:G:39:ARG:HB3	1:G:49:ILE:HD11	1.65	0.78
2:H:30:ILE:HD12	2:H:30:ILE:H	1.48	0.77
2:F:130:VAL:HG11	2:F:160:PHE:HB3	1.66	0.77
1:C:22:ARG:HG2	1:C:76:VAL:HG12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:VAL:HG11	2:H:160:PHE:HB3	1.67	0.76
2:H:209:ARG:HD2	2:H:224:GLU:HG2	1.67	0.76
1:G:22:ARG:HG2	1:G:76:VAL:HG12	1.68	0.75
1:A:36:ASN:HD21	1:A:51:ARG:NH1	1.83	0.75
1:E:158:LYS:HE2	1:E:184:GLU:HG3	1.70	0.74
2:D:30:ILE:HD12	2:D:30:ILE:H	1.53	0.74
2:F:171:LYS:HD2	2:F:172:LYS:HG3	1.70	0.74
2:B:156:LEU:HD12	2:B:166:ILE:HD11	1.70	0.73
2:B:187:THR:O	2:B:190:THR:HG22	1.89	0.73
2:F:130:VAL:HG13	2:F:160:PHE:N	2.03	0.72
1:C:122:GLN:HB2	1:C:123:PRO:HD2	1.72	0.72
2:H:187:THR:O	2:H:190:THR:HG22	1.88	0.72
1:C:36:ASN:HD21	1:C:51:ARG:NH1	1.88	0.72
2:D:130:VAL:HG11	2:D:160:PHE:HB3	1.70	0.72
1:C:36:ASN:ND2	1:C:51:ARG:HH11	1.88	0.71
2:B:185:MET:CE	4:B:2004:HOH:O	2.38	0.71
2:H:130:VAL:HG13	2:H:160:PHE:N	2.06	0.71
2:D:130:VAL:HG13	2:D:160:PHE:N	2.05	0.71
2:H:126:LEU:HD13	2:H:126:LEU:H	1.54	0.70
1:A:40:LYS:HG2	1:A:46:MET:H	1.56	0.70
2:F:187:THR:O	2:F:190:THR:HG22	1.90	0.70
2:B:130:VAL:HG11	2:B:160:PHE:HB3	1.72	0.70
1:E:99:MET:HE3	1:E:100:GLY:H	1.57	0.70
1:G:164:ASP:H	2:H:185:MET:HE1	1.56	0.70
2:H:9:ILE:CG2	2:H:163:VAL:HG12	2.22	0.69
2:B:34:SER:OG	2:B:53:SER:HA	1.91	0.69
1:E:2:ILE:HD11	1:E:25:MET:HE2	1.74	0.69
2:D:103:GLN:HB3	2:D:104:GLN:OE1	1.93	0.69
2:F:9:ILE:CG2	2:F:163:VAL:HG12	2.23	0.68
1:C:72:LYS:HA	1:C:72:LYS:HE2	1.74	0.68
1:G:40:LYS:HG2	1:G:46:MET:H	1.58	0.68
1:A:122:GLN:HE22	1:A:174:LYS:HG2	1.59	0.67
1:C:144:GLU:OE1	1:C:174:LYS:HD2	1.95	0.67
2:H:156:LEU:HD12	2:H:166:ILE:HD11	1.76	0.67
2:D:187:THR:O	2:D:190:THR:HG22	1.95	0.67
2:B:130:VAL:HG13	2:B:160:PHE:N	2.10	0.67
1:C:95:ASP:HB3	1:C:107:LEU:HD23	1.76	0.67
1:E:36:ASN:HD21	1:E:51:ARG:HH11	1.43	0.67
2:B:30:ILE:H	2:B:30:ILE:CD1	2.01	0.67
2:D:137:PHE:HB2	2:D:153:LEU:O	1.94	0.67
1:E:99:MET:HG3	1:E:101:GLY:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:GLU:OE1	1:E:174:LYS:HD2	1.96	0.66
2:D:144:THR:O	2:D:148:LYS:HA	1.95	0.66
1:E:163:PHE:HB3	2:F:185:MET:HE1	1.77	0.66
2:D:15:LEU:HD12	2:D:15:LEU:H	1.59	0.66
2:F:156:LEU:HD12	2:F:166:ILE:HD11	1.76	0.66
1:E:40:LYS:HG2	1:E:46:MET:H	1.61	0.66
1:C:2:ILE:HD12	1:C:33:TYR:CE2	2.31	0.66
2:B:209:ARG:NH1	2:B:226:ILE:HG12	2.11	0.65
1:C:40:LYS:HG2	1:C:46:MET:H	1.61	0.65
1:C:22:ARG:HB3	1:C:74:LEU:HD21	1.79	0.65
1:E:154:LEU:HD13	1:E:183:TYR:OH	1.97	0.65
2:H:74:ILE:HD12	2:H:74:ILE:H	1.60	0.65
2:D:77:THR:OG1	2:D:79:THR:HG23	1.96	0.65
2:B:144:THR:O	2:B:148:LYS:HA	1.95	0.65
2:F:15:LEU:HD12	2:F:15:LEU:H	1.60	0.65
1:A:49:ILE:HG23	1:A:60:PHE:CD2	2.32	0.65
2:F:179:SER:HB3	2:F:197:LEU:HD13	1.78	0.65
2:H:30:ILE:HG22	2:H:73:ARG:HH21	1.61	0.64
2:H:73:ARG:O	2:H:73:ARG:HD3	1.97	0.64
2:H:144:THR:O	2:H:148:LYS:HA	1.97	0.64
2:D:5:GLU:HB2	2:D:24:VAL:HG22	1.78	0.64
2:F:126:LEU:HD12	2:F:126:LEU:H	1.61	0.64
1:G:99:MET:HE3	1:G:100:GLY:N	2.12	0.64
1:E:102:GLU:H	1:E:102:GLU:CD	2.05	0.64
2:F:124:LYS:HZ1	1:G:120:ARG:HG2	1.62	0.64
2:F:144:THR:O	2:F:148:LYS:HA	1.98	0.64
2:B:15:LEU:H	2:B:15:LEU:HD12	1.62	0.64
2:F:130:VAL:O	2:F:159:PHE:HA	1.97	0.64
2:H:103:GLN:HB2	2:H:108:LYS:O	1.98	0.64
1:G:164:ASP:N	2:H:185:MET:HE1	2.13	0.63
1:C:163:PHE:HB3	2:D:185:MET:HE1	1.80	0.63
1:C:124:HIS:HD1	1:C:196:ASP:CG	2.06	0.63
2:B:77:THR:O	2:B:79:THR:HG22	1.98	0.63
2:D:4:LEU:HD22	2:D:25:VAL:HG12	1.80	0.63
2:H:99:LEU:HD23	2:H:99:LEU:O	1.98	0.63
1:A:34:TYR:HE1	1:A:97:LEU:HB3	1.64	0.63
2:H:15:LEU:HD12	2:H:15:LEU:H	1.64	0.63
2:H:5:GLU:HB2	2:H:24:VAL:HG22	1.80	0.63
2:D:87:VAL:HG21	2:D:121:ILE:HD11	1.80	0.63
1:E:120:ARG:NH1	1:E:120:ARG:HB3	2.14	0.63
1:G:49:ILE:HG23	1:G:60:PHE:CD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:GLU:OE1	1:A:174:LYS:HD2	1.99	0.62
1:C:154:LEU:HD13	1:C:183:TYR:OH	1.98	0.62
2:B:24:VAL:HG23	2:B:24:VAL:O	1.99	0.62
2:B:87:VAL:HG21	2:B:121:ILE:HD11	1.82	0.62
1:A:143:LYS:NZ	2:B:146:LEU:HD23	2.15	0.62
2:D:179:SER:HB3	2:D:197:LEU:HD13	1.81	0.62
1:E:137:ASN:HD21	1:E:182:LYS:HZ3	1.46	0.62
2:F:137:PHE:HB2	2:F:153:LEU:O	1.99	0.62
2:H:130:VAL:O	2:H:159:PHE:HA	1.99	0.62
1:E:105:ASP:HB2	2:F:36:TYR:OH	1.99	0.62
1:C:69:ASP:OD1	1:C:71:ALA:HB3	2.00	0.62
2:D:9:ILE:CG2	2:D:163:VAL:HG12	2.29	0.62
2:D:214:HIS:CD2	2:D:216:ASN:H	2.18	0.62
1:E:74:LEU:HD12	1:E:75:ALA:N	2.14	0.62
1:E:38:TYR:OH	2:F:111:LYS:HB3	1.99	0.61
1:G:144:GLU:OE1	1:G:174:LYS:HD2	1.99	0.61
1:C:49:ILE:HG23	1:C:60:PHE:CD2	2.35	0.61
2:D:210:CYS:HB3	2:D:225:ILE:HB	1.82	0.61
1:G:2:ILE:HD12	1:G:33:TYR:CZ	2.35	0.61
1:A:163:PHE:HB3	2:B:185:MET:HE1	1.82	0.61
2:F:161:PRO:HD2	2:F:214:HIS:NE2	2.15	0.61
2:B:33:THR:HG22	2:B:34:SER:N	2.16	0.61
2:B:214:HIS:CD2	2:B:216:ASN:H	2.19	0.61
2:D:130:VAL:O	2:D:159:PHE:HA	2.01	0.61
2:F:16:SER:OG	1:G:80:LEU:HB2	2.01	0.61
2:F:156:LEU:HD12	2:F:166:ILE:CD1	2.31	0.61
1:E:99:MET:HE3	1:E:100:GLY:N	2.16	0.60
2:B:130:VAL:O	2:B:159:PHE:HA	2.01	0.60
2:D:30:ILE:HD12	2:D:30:ILE:N	2.15	0.60
2:H:137:PHE:HB2	2:H:153:LEU:O	2.00	0.60
2:B:179:SER:HB3	2:B:197:LEU:HD13	1.82	0.60
1:C:135:GLY:C	1:C:137:ASN:H	2.10	0.60
1:C:2:ILE:HD11	1:C:25:MET:HE2	1.82	0.60
2:F:214:HIS:CD2	2:F:216:ASN:H	2.19	0.60
2:B:137:PHE:HB2	2:B:153:LEU:O	2.02	0.60
2:F:5:GLU:HB2	2:F:24:VAL:HG22	1.83	0.60
2:H:162:ASP:OD2	2:H:162:ASP:C	2.45	0.60
2:H:214:HIS:CD2	2:H:216:ASN:H	2.19	0.60
2:B:170:GLU:HB2	2:B:173:SER:O	2.01	0.60
2:B:5:GLU:HB2	2:B:24:VAL:HG22	1.83	0.60
1:G:55:ILE:HD11	2:H:108:LYS:HD2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:THR:HG21	1:G:194:GLN:OE1	2.02	0.59
1:E:120:ARG:HB3	1:E:120:ARG:HH11	1.67	0.59
1:A:36:ASN:ND2	1:A:51:ARG:HH11	1.88	0.59
2:F:130:VAL:CG1	2:F:160:PHE:HB3	2.31	0.59
1:G:35:ILE:HD12	1:G:94:CYS:SG	2.43	0.59
2:B:209:ARG:HH12	2:B:226:ILE:HG12	1.67	0.59
2:F:137:PHE:CD2	2:F:153:LEU:HD23	2.38	0.59
1:C:103:TYR:HD2	1:C:103:TYR:H	1.49	0.59
2:B:161:PRO:HD2	2:B:214:HIS:NE2	2.18	0.59
1:C:55:ILE:HG12	2:D:108:LYS:HE3	1.84	0.59
2:B:99:LEU:O	2:B:99:LEU:HD23	2.03	0.58
2:H:156:LEU:HD12	2:H:166:ILE:CD1	2.32	0.58
1:A:42:GLN:O	1:A:42:GLN:HG3	2.04	0.58
2:B:60:LYS:HD2	2:B:64:ILE:HB	1.86	0.58
2:D:156:LEU:HD12	2:D:166:ILE:HD11	1.84	0.58
1:E:135:GLY:C	1:E:137:ASN:H	2.12	0.58
1:G:7:GLU:HG2	1:G:8:HIS:CE1	2.39	0.58
2:B:31:SER:O	2:B:32:ALA:HB2	2.04	0.58
2:D:161:PRO:HD2	2:D:214:HIS:NE2	2.18	0.58
1:E:36:ASN:HD21	1:E:51:ARG:NH1	2.02	0.58
1:G:34:TYR:HD2	1:G:52:GLU:HG2	1.68	0.58
1:C:120:ARG:HG2	1:C:120:ARG:HH11	1.69	0.58
2:H:130:VAL:CG1	2:H:160:PHE:HB3	2.33	0.58
1:A:30:ILE:H	1:A:73:ASN:CG	2.11	0.58
2:D:103:GLN:HB2	2:D:108:LYS:HB3	1.85	0.58
1:E:122:GLN:HB2	1:E:123:PRO:HD2	1.86	0.58
1:A:135:GLY:C	1:A:137:ASN:H	2.11	0.58
1:G:137:ASN:HD21	1:G:182:LYS:HZ3	1.52	0.58
2:F:173:SER:O	2:F:175:THR:HG23	2.04	0.57
1:A:150:ILE:HD11	1:A:193:VAL:HG11	1.86	0.57
1:E:42:GLN:O	1:E:42:GLN:HG3	2.05	0.57
2:B:2:GLY:HA3	2:B:28:ILE:HG12	1.85	0.57
2:B:74:ILE:HD12	2:B:74:ILE:N	2.20	0.57
1:C:74:LEU:HD23	1:C:75:ALA:N	2.19	0.57
1:E:49:ILE:HG23	1:E:60:PHE:CD2	2.39	0.57
1:G:135:GLY:C	1:G:137:ASN:H	2.12	0.57
2:D:169:GLU:OE1	2:D:174:ASN:HB2	2.05	0.57
4:E:2030:HOH:O	2:F:185:MET:CE	2.52	0.57
1:G:150:ILE:HD11	1:G:193:VAL:HG11	1.86	0.57
2:B:130:VAL:CG1	2:B:160:PHE:HB3	2.33	0.57
1:A:29:ALA:HA	1:A:73:ASN:HD21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:130:VAL:CG1	2:F:160:PHE:H	2.13	0.57
2:B:9:ILE:CG2	2:B:163:VAL:HG12	2.35	0.57
1:E:20:THR:HG22	1:E:78:LYS:HG3	1.86	0.57
2:H:87:VAL:HG21	2:H:121:ILE:HD11	1.87	0.57
2:H:99:LEU:HD23	2:H:99:LEU:C	2.29	0.57
2:D:130:VAL:O	2:D:130:VAL:CG1	2.53	0.56
1:G:136:THR:HA	1:G:186:SER:HB3	1.87	0.56
1:A:119:PRO:HB3	1:A:173:GLY:O	2.06	0.56
2:B:156:LEU:HD12	2:B:166:ILE:CD1	2.35	0.56
1:E:168:VAL:HG12	1:E:169:ILE:N	2.21	0.56
2:F:87:VAL:HG21	2:F:121:ILE:HD11	1.86	0.56
2:H:179:SER:HB3	2:H:197:LEU:HD13	1.85	0.56
1:A:164:ASP:H	2:B:185:MET:HE1	1.69	0.56
1:G:154:LEU:HD13	1:G:183:TYR:OH	2.05	0.56
1:A:122:GLN:HB2	1:A:123:PRO:CD	2.32	0.56
2:D:156:LEU:HD12	2:D:166:ILE:CD1	2.36	0.55
4:E:2030:HOH:O	2:F:185:MET:HE2	2.05	0.55
2:D:201:GLU:O	2:D:204:LEU:HD13	2.07	0.55
1:A:107:LEU:HD11	2:B:111:LYS:HD3	1.88	0.55
2:B:55:ASP:N	2:B:55:ASP:OD2	2.39	0.55
2:H:177:LEU:N	2:H:177:LEU:HD12	2.22	0.55
2:B:185:MET:HE2	4:B:2004:HOH:O	2.06	0.55
2:B:185:MET:HE3	4:B:2004:HOH:O	2.03	0.55
2:F:210:CYS:HB3	2:F:225:ILE:HB	1.88	0.55
1:G:143:LYS:NZ	2:H:146:LEU:HD23	2.22	0.55
2:F:201:GLU:O	2:F:204:LEU:HD13	2.07	0.55
2:F:9:ILE:HG22	2:F:163:VAL:HG12	1.89	0.54
1:G:168:VAL:HG12	1:G:169:ILE:N	2.22	0.54
1:A:34:TYR:CE1	1:A:97:LEU:HB3	2.42	0.54
2:B:24:VAL:O	2:B:24:VAL:CG2	2.56	0.54
2:D:77:THR:HA	1:G:153:ASN:ND2	2.23	0.54
2:F:99:LEU:HD23	2:F:99:LEU:O	2.07	0.54
2:B:141:ILE:HG22	2:B:145:LYS:HE3	1.88	0.54
2:D:70:GLU:HB2	2:D:83:THR:HB	1.89	0.54
1:G:35:ILE:H	1:G:52:GLU:HB2	1.73	0.54
2:B:137:PHE:CD2	2:B:153:LEU:HD23	2.41	0.54
2:D:130:VAL:CG1	2:D:160:PHE:HB3	2.36	0.54
2:B:171:LYS:HD3	2:B:171:LYS:C	2.33	0.54
2:F:177:LEU:HD12	2:F:177:LEU:N	2.23	0.54
2:H:9:ILE:HG22	2:H:163:VAL:HG12	1.90	0.54
2:H:210:CYS:HB3	2:H:225:ILE:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:THR:HA	1:C:186:SER:HB3	1.90	0.54
2:B:130:VAL:O	2:B:130:VAL:CG1	2.56	0.54
1:E:136:THR:HA	1:E:186:SER:HB3	1.89	0.54
1:C:105:ASP:HB3	2:D:36:TYR:OH	2.09	0.53
2:F:30:ILE:N	2:F:30:ILE:HD12	2.23	0.53
1:E:32:ASN:O	1:E:97:LEU:HB2	2.09	0.53
1:A:122:GLN:NE2	1:A:174:LYS:HG2	2.22	0.53
2:B:99:LEU:HD23	2:B:99:LEU:C	2.33	0.53
1:C:102:GLU:CD	1:C:102:GLU:H	2.15	0.53
1:C:150:ILE:HD11	1:C:193:VAL:HG11	1.90	0.53
1:A:136:THR:HA	1:A:186:SER:HB3	1.90	0.53
1:C:42:GLN:O	1:C:42:GLN:HG3	2.08	0.53
1:E:150:ILE:HD11	1:E:193:VAL:HG11	1.91	0.53
2:D:170:GLU:HB2	2:D:173:SER:O	2.09	0.53
1:E:20:THR:HG22	1:E:78:LYS:CG	2.39	0.53
1:E:119:PRO:HD2	1:E:175:TYR:OH	2.08	0.53
2:B:177:LEU:N	2:B:177:LEU:HD12	2.24	0.53
2:B:209:ARG:HG2	2:B:209:ARG:HH11	1.73	0.53
2:D:99:LEU:HD23	2:D:99:LEU:O	2.09	0.53
2:H:54:TYR:C	2:H:56:GLY:H	2.17	0.53
2:H:171:LYS:HA	2:H:209:ARG:NH2	2.12	0.53
2:B:210:CYS:HB3	2:B:225:ILE:HB	1.90	0.53
2:H:70:GLU:HB2	2:H:83:THR:HB	1.90	0.53
1:E:28:GLU:HG2	1:E:29:ALA:H	1.73	0.52
2:D:162:ASP:OD2	2:D:162:ASP:C	2.52	0.52
2:F:160:PHE:O	2:F:161:PRO:C	2.52	0.52
2:B:30:ILE:HG22	2:B:73:ARG:HH21	1.75	0.52
2:B:160:PHE:O	2:B:161:PRO:C	2.52	0.52
1:G:2:ILE:HD13	1:G:108:ILE:HD12	1.89	0.52
2:B:100:TRP:CZ2	2:B:111:LYS:HD2	2.44	0.52
1:C:99:MET:HE3	1:C:100:GLY:H	1.75	0.52
2:D:137:PHE:CD2	2:D:153:LEU:HD23	2.44	0.52
1:A:168:VAL:HG12	1:A:169:ILE:N	2.25	0.52
2:D:34:SER:OG	2:D:53:SER:HA	2.09	0.52
1:G:158:LYS:HB2	1:G:184:GLU:HB2	1.92	0.52
1:A:143:LYS:HZ3	2:B:146:LEU:HD23	1.74	0.52
1:A:158:LYS:HB2	1:A:184:GLU:HB2	1.92	0.52
2:H:201:GLU:O	2:H:204:LEU:HD13	2.10	0.52
2:H:209:ARG:HG3	2:H:209:ARG:HH11	1.74	0.52
1:A:35:ILE:HG21	1:A:75:ALA:HB1	1.92	0.52
2:D:104:GLN:HG2	2:D:105:GLU:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:PHE:HB3	2:H:185:MET:HE1	1.90	0.52
1:A:154:LEU:HD13	1:A:183:TYR:OH	2.09	0.52
1:G:42:GLN:HG3	1:G:42:GLN:O	2.10	0.52
2:D:28:ILE:HD12	2:D:101:GLU:HG3	1.92	0.51
1:E:22:ARG:HG2	1:E:74:LEU:HD11	1.91	0.51
2:F:60:LYS:HD2	2:F:64:ILE:HB	1.93	0.51
2:F:24:VAL:O	2:F:24:VAL:HG23	2.10	0.51
2:H:160:PHE:O	2:H:161:PRO:C	2.53	0.51
1:C:168:VAL:HG12	1:C:169:ILE:N	2.25	0.51
2:D:146:LEU:C	2:D:148:LYS:H	2.18	0.51
1:G:63:ASN:O	1:G:80:LEU:HG	2.11	0.51
2:H:161:PRO:HD2	2:H:214:HIS:NE2	2.26	0.51
2:D:103:GLN:HB2	2:D:108:LYS:CB	2.41	0.51
2:F:70:GLU:HB2	2:F:83:THR:HB	1.92	0.51
2:D:130:VAL:CG1	2:D:160:PHE:H	2.15	0.51
2:D:177:LEU:HD12	2:D:177:LEU:N	2.25	0.51
2:H:60:LYS:HD2	2:H:64:ILE:HB	1.93	0.51
1:A:7:GLU:HG2	1:A:8:HIS:CE1	2.46	0.50
2:B:162:ASP:OD2	2:B:162:ASP:C	2.54	0.50
1:E:51:ARG:HH11	1:E:51:ARG:HG3	1.77	0.50
2:H:21:LEU:CD1	2:H:21:LEU:N	2.74	0.50
2:H:171:LYS:HB2	2:H:209:ARG:HH12	1.76	0.50
2:B:201:GLU:O	2:B:204:LEU:HD13	2.12	0.50
2:D:160:PHE:O	2:D:161:PRO:C	2.53	0.50
1:G:164:ASP:HB2	2:H:185:MET:HE2	1.93	0.50
1:C:120:ARG:HG2	1:C:120:ARG:NH1	2.26	0.50
2:B:168:TRP:O	2:B:169:GLU:HG3	2.12	0.50
2:B:171:LYS:HG2	2:B:209:ARG:NH2	2.27	0.50
2:F:75:PRO:HG2	2:F:76:GLU:OE1	2.11	0.50
2:H:130:VAL:CG1	2:H:160:PHE:H	2.17	0.49
1:C:48:PHE:CE2	2:D:110:ILE:HD13	2.46	0.49
1:E:103:TYR:H	1:E:103:TYR:HD2	1.60	0.49
1:E:137:ASN:HB3	2:F:137:PHE:HZ	1.78	0.49
1:G:15:ILE:HD11	1:G:169:ILE:HG21	1.93	0.49
1:G:137:ASN:HD21	1:G:182:LYS:NZ	2.10	0.49
2:F:126:LEU:HD12	2:F:126:LEU:N	2.26	0.49
1:G:35:ILE:CD1	1:G:94:CYS:SG	3.00	0.49
1:A:164:ASP:N	2:B:185:MET:HE1	2.26	0.49
2:D:77:THR:O	2:D:79:THR:HG22	2.12	0.49
2:D:60:LYS:HD2	2:D:64:ILE:HB	1.95	0.49
2:F:9:ILE:HG22	2:F:163:VAL:CG1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:GLU:HB2	2:B:83:THR:HB	1.93	0.49
2:F:162:ASP:C	2:F:162:ASP:OD2	2.56	0.49
2:H:160:PHE:HB3	2:H:161:PRO:HD3	1.94	0.49
1:C:51:ARG:HH11	1:C:51:ARG:HG3	1.77	0.49
1:E:105:ASP:HB3	2:F:100:TRP:NE1	2.28	0.49
2:D:38:TYR:OH	2:D:111:LYS:NZ	2.41	0.49
2:B:21:LEU:CD1	2:B:21:LEU:N	2.76	0.48
2:F:37:TRP:O	2:F:49:LEU:HB3	2.13	0.48
1:A:102:GLU:CD	1:A:102:GLU:H	2.20	0.48
1:C:22:ARG:CB	1:C:74:LEU:HD21	2.43	0.48
2:F:146:LEU:C	2:F:148:LYS:H	2.21	0.48
1:G:122:GLN:HB2	1:G:123:PRO:CD	2.42	0.48
1:A:137:ASN:HB3	2:B:137:PHE:CZ	2.48	0.48
2:D:91:ASP:O	2:D:119:LEU:HD23	2.13	0.48
2:D:104:GLN:CD	2:D:104:GLN:H	2.21	0.48
1:E:36:ASN:ND2	1:E:51:ARG:HH11	2.10	0.48
1:E:18:PRO:HG3	1:E:80:LEU:O	2.14	0.48
2:B:169:GLU:OE1	2:B:174:ASN:HB2	2.14	0.48
2:F:73:ARG:O	2:F:73:ARG:HG3	2.14	0.48
2:H:171:LYS:HD3	2:H:209:ARG:NH1	2.28	0.48
2:D:21:LEU:N	2:D:21:LEU:CD1	2.77	0.48
2:B:146:LEU:C	2:B:148:LYS:H	2.20	0.48
1:E:51:ARG:HB3	1:E:55:ILE:HB	1.96	0.48
2:F:16:SER:OG	1:G:80:LEU:CB	2.62	0.48
2:H:130:VAL:O	2:H:130:VAL:CG1	2.62	0.48
2:D:30:ILE:H	2:D:30:ILE:CD1	2.25	0.47
1:G:124:HIS:CD2	1:G:147:PRO:HD3	2.49	0.47
2:H:137:PHE:CD2	2:H:153:LEU:HD23	2.49	0.47
1:C:166:ALA:O	1:C:177:ALA:HA	2.14	0.47
1:E:137:ASN:HD21	1:E:182:LYS:NZ	2.12	0.47
1:G:166:ALA:O	1:G:177:ALA:HA	2.14	0.47
2:H:146:LEU:C	2:H:148:LYS:H	2.20	0.47
2:H:209:ARG:HD2	2:H:224:GLU:CG	2.40	0.47
1:A:15:ILE:HD11	1:A:169:ILE:HG21	1.96	0.47
1:E:105:ASP:HB3	2:F:100:TRP:HE1	1.79	0.47
2:F:28:ILE:HG22	2:F:29:THR:N	2.30	0.47
2:B:33:THR:HG22	2:B:34:SER:H	1.79	0.47
2:D:73:ARG:O	2:D:73:ARG:HG3	2.13	0.47
1:E:53:LYS:O	1:E:55:ILE:HG13	2.14	0.47
1:C:7:GLU:HG2	1:C:8:HIS:CE1	2.49	0.47
2:D:31:SER:O	2:D:32:ALA:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ALA:O	1:A:177:ALA:HA	2.15	0.47
2:F:130:VAL:O	2:F:130:VAL:CG1	2.63	0.47
2:F:145:LYS:HB2	4:F:2002:HOH:O	2.15	0.47
2:H:37:TRP:O	2:H:49:LEU:HB3	2.15	0.47
2:H:141:ILE:HG22	2:H:145:LYS:HE3	1.96	0.47
2:B:14:THR:O	2:B:17:LYS:HB2	2.15	0.47
2:B:91:ASP:O	2:B:119:LEU:HD23	2.15	0.47
2:F:4:LEU:HD22	2:F:25:VAL:HG12	1.97	0.47
2:F:15:LEU:HD12	2:F:15:LEU:N	2.28	0.47
2:F:24:VAL:O	2:F:24:VAL:CG2	2.63	0.47
1:G:53:LYS:HA	1:G:53:LYS:HD3	1.58	0.47
1:G:180:LEU:HD11	2:H:153:LEU:HD21	1.97	0.47
2:H:160:PHE:O	2:H:162:ASP:N	2.48	0.47
2:H:9:ILE:HG22	2:H:163:VAL:CG1	2.45	0.47
1:A:117:VAL:O	1:A:169:ILE:HD11	2.15	0.46
2:B:9:ILE:HG22	2:B:163:VAL:HG12	1.96	0.46
1:C:137:ASN:HD21	1:C:182:LYS:NZ	2.13	0.46
2:B:15:LEU:H	2:B:15:LEU:CD1	2.28	0.46
2:D:13:LYS:O	2:D:121:ILE:HA	2.15	0.46
1:G:137:ASN:HB3	2:H:137:PHE:CZ	2.50	0.46
2:H:169:GLU:HG3	2:H:211:ILE:HD12	1.97	0.46
2:F:52:ILE:HG23	2:F:52:ILE:O	2.16	0.46
2:F:126:LEU:H	2:F:126:LEU:CD1	2.27	0.46
1:G:119:PRO:HD2	1:G:175:TYR:OH	2.16	0.46
2:H:4:LEU:HD22	2:H:25:VAL:HG12	1.97	0.46
2:F:141:ILE:HG22	2:F:145:LYS:HE3	1.96	0.46
2:H:73:ARG:O	2:H:75:PRO:HD3	2.15	0.46
2:F:53:SER:HB3	2:F:55:ASP:OD2	2.15	0.46
1:G:72:LYS:HE2	1:G:72:LYS:HA	1.95	0.46
1:G:122:GLN:HE22	1:G:174:LYS:HG2	1.81	0.46
1:G:143:LYS:HZ3	2:H:146:LEU:HD23	1.80	0.46
2:H:91:ASP:O	2:H:119:LEU:HD23	2.16	0.46
1:C:137:ASN:HD21	1:C:182:LYS:HZ3	1.63	0.46
1:E:7:GLU:HG2	1:E:8:HIS:CE1	2.51	0.46
2:B:28:ILE:HD11	2:B:101:GLU:OE1	2.16	0.46
2:B:4:LEU:HD11	2:B:99:LEU:HD22	1.97	0.46
1:G:134:ASN:O	1:G:137:ASN:HB2	2.16	0.46
1:G:136:THR:O	1:G:182:LYS:HA	2.14	0.46
2:H:2:GLY:HA3	2:H:28:ILE:HG12	1.97	0.46
2:B:37:TRP:O	2:B:49:LEU:HB3	2.16	0.46
1:E:99:MET:HB3	1:E:103:TYR:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:ALA:O	1:E:177:ALA:HA	2.15	0.46
1:E:99:MET:HG3	1:E:101:GLY:N	2.29	0.46
1:E:99:MET:C	1:E:101:GLY:H	2.24	0.46
1:A:127:PRO:HD3	1:A:195:HIS:CD2	2.51	0.45
2:B:169:GLU:HA	2:B:177:LEU:CD1	2.46	0.45
2:B:74:ILE:N	2:B:74:ILE:CD1	2.79	0.45
1:C:203:THR:C	1:C:205:PHE:H	2.25	0.45
2:D:15:LEU:HD12	2:D:15:LEU:N	2.29	0.45
2:D:24:VAL:HG23	2:D:24:VAL:O	2.14	0.45
1:E:67:ASP:O	1:E:76:VAL:HG22	2.17	0.45
1:G:127:PRO:HD3	1:G:195:HIS:CD2	2.51	0.45
2:B:100:TRP:CE2	2:B:111:LYS:HD2	2.50	0.45
2:H:52:ILE:HG23	2:H:52:ILE:O	2.16	0.45
2:H:24:VAL:O	2:H:24:VAL:HG23	2.17	0.45
2:B:73:ARG:O	2:B:73:ARG:HD3	2.17	0.45
2:F:21:LEU:N	2:F:21:LEU:CD1	2.80	0.45
1:E:98:GLY:HA2	1:E:103:TYR:CE1	2.52	0.45
1:E:137:ASN:HB3	2:F:137:PHE:CZ	2.52	0.45
1:A:20:THR:CG2	1:A:78:LYS:HG3	2.39	0.45
1:A:122:GLN:HE22	1:A:174:LYS:HE2	1.82	0.45
1:E:99:MET:HB3	1:E:103:TYR:CD2	2.52	0.45
1:E:134:ASN:O	1:E:137:ASN:HB2	2.16	0.45
1:C:135:GLY:C	1:C:137:ASN:N	2.75	0.45
2:D:141:ILE:HG22	2:D:145:LYS:HE3	1.99	0.44
1:E:25:MET:HE1	1:E:33:TYR:CD2	2.52	0.44
1:E:34:TYR:HB2	1:E:95:ASP:OD1	2.18	0.44
2:B:73:ARG:O	2:B:75:PRO:HD3	2.18	0.44
2:B:171:LYS:HB2	2:B:207:GLU:HB3	2.00	0.44
2:D:37:TRP:O	2:D:49:LEU:HB3	2.17	0.44
2:H:4:LEU:HD11	2:H:99:LEU:HD22	1.99	0.44
2:H:13:LYS:O	2:H:121:ILE:HA	2.17	0.44
2:B:8:GLN:OE1	2:B:21:LEU:HA	2.17	0.44
2:B:13:LYS:O	2:B:121:ILE:HA	2.17	0.44
2:F:13:LYS:O	2:F:121:ILE:HA	2.17	0.44
1:A:136:THR:HA	1:A:183:TYR:O	2.18	0.44
2:H:77:THR:O	2:H:79:THR:HG22	2.17	0.44
2:B:171:LYS:HG3	2:B:207:GLU:OE2	2.17	0.44
1:C:18:PRO:HG3	1:C:80:LEU:O	2.18	0.44
2:H:53:SER:HB2	2:H:55:ASP:OD2	2.18	0.44
2:B:15:LEU:HD12	2:B:15:LEU:N	2.30	0.44
2:B:146:LEU:HG	2:B:147:GLN:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:137:ASN:HB3	2:H:137:PHE:HZ	1.83	0.44
1:A:69:ASP:OD1	1:A:71:ALA:HB3	2.18	0.43
1:C:67:ASP:O	1:C:76:VAL:HG22	2.18	0.43
1:G:164:ASP:H	2:H:185:MET:CE	2.26	0.43
1:C:136:THR:HA	1:C:183:TYR:O	2.18	0.43
2:D:61:GLU:HG3	2:D:62:SER:N	2.32	0.43
2:D:210:CYS:SG	2:D:225:ILE:HD12	2.58	0.43
2:F:160:PHE:O	2:F:162:ASP:N	2.51	0.43
2:H:209:ARG:HG3	2:H:209:ARG:NH1	2.33	0.43
2:F:4:LEU:HD11	2:F:99:LEU:HD22	2.01	0.43
1:G:30:ILE:HD11	1:G:35:ILE:CD1	2.44	0.43
1:A:107:LEU:HD21	2:B:100:TRP:CZ2	2.53	0.43
1:A:137:ASN:HB3	2:B:137:PHE:HZ	1.83	0.43
2:B:136:ILE:HG23	2:B:227:PHE:CE1	2.54	0.43
2:D:13:LYS:HD2	2:D:17:LYS:HE2	2.00	0.43
2:H:30:ILE:HB	2:H:31:SER:H	1.61	0.43
1:G:34:TYR:CD2	1:G:52:GLU:HG2	2.52	0.43
2:H:17:LYS:HG3	2:H:18:THR:H	1.82	0.43
1:A:20:THR:HG22	1:A:78:LYS:CG	2.42	0.43
1:C:136:THR:O	1:C:182:LYS:HA	2.18	0.43
2:D:8:GLN:OE1	2:D:21:LEU:HA	2.19	0.43
1:E:32:ASN:HA	1:E:97:LEU:HD12	1.99	0.43
2:H:140:SER:O	2:H:141:ILE:C	2.61	0.43
1:E:74:LEU:HD12	1:E:75:ALA:H	1.79	0.43
2:B:12:THR:O	2:B:13:LYS:HD3	2.18	0.43
2:D:218:LYS:O	2:D:219:ASN:HB2	2.18	0.43
2:H:144:THR:HA	2:H:149:ALA:O	2.19	0.43
2:B:77:THR:O	2:B:78:SER:C	2.62	0.43
1:E:70:ILE:H	1:E:70:ILE:HG13	1.52	0.43
1:E:127:PRO:HD3	1:E:195:HIS:CD2	2.54	0.43
1:E:136:THR:O	1:E:182:LYS:HA	2.18	0.43
1:G:55:ILE:CG2	2:H:110:ILE:HD11	2.49	0.43
1:A:99:MET:HB3	1:A:103:TYR:HB3	2.00	0.43
2:B:33:THR:CG2	2:B:34:SER:N	2.82	0.43
2:D:14:THR:OG1	2:D:17:LYS:HD3	2.19	0.43
2:F:99:LEU:HD23	2:F:99:LEU:C	2.44	0.43
2:H:104:GLN:HB2	2:H:105:GLU:OE1	2.19	0.42
2:H:213:ARG:HE	2:H:222:ASP:CG	2.27	0.42
2:D:12:THR:O	2:D:13:LYS:HD3	2.19	0.42
1:A:135:GLY:C	1:A:137:ASN:N	2.76	0.42
2:B:73:ARG:HH11	2:B:73:ARG:HG2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:LEU:HD12	2:B:107:GLY:N	2.34	0.42
2:B:160:PHE:HB3	2:B:161:PRO:HD3	2.01	0.42
1:E:52:GLU:O	1:E:53:LYS:HB2	2.19	0.42
1:A:180:LEU:HD11	2:B:153:LEU:HD21	2.01	0.42
1:E:28:GLU:HG2	1:E:29:ALA:N	2.34	0.42
1:E:143:LYS:NZ	2:F:146:LEU:HD23	2.35	0.42
1:E:203:THR:C	1:E:205:PHE:H	2.27	0.42
2:F:27:GLY:O	2:F:28:ILE:HD13	2.18	0.42
2:F:85:HIS:O	2:F:86:ASN:C	2.61	0.42
2:F:145:LYS:HD2	2:F:145:LYS:N	2.33	0.42
1:G:203:THR:C	1:G:205:PHE:H	2.26	0.42
1:A:18:PRO:HG3	1:A:80:LEU:O	2.20	0.42
2:B:160:PHE:O	2:B:162:ASP:N	2.52	0.42
2:B:171:LYS:HD3	2:B:172:LYS:N	2.35	0.42
1:C:70:ILE:O	1:C:70:ILE:HG12	2.18	0.42
2:F:171:LYS:HD2	2:F:172:LYS:HZ2	1.85	0.42
1:A:30:ILE:HG22	1:A:73:ASN:OD1	2.20	0.42
2:B:145:LYS:N	2:B:145:LYS:HD2	2.34	0.42
1:C:8:HIS:O	1:C:113:THR:HB	2.19	0.42
1:C:127:PRO:HD3	1:C:195:HIS:CD2	2.55	0.42
2:F:15:LEU:H	2:F:15:LEU:CD1	2.28	0.42
2:F:8:GLN:OE1	2:F:21:LEU:HA	2.20	0.42
1:G:136:THR:HA	1:G:183:TYR:O	2.19	0.42
1:A:35:ILE:HD12	1:A:35:ILE:N	2.34	0.42
2:B:144:THR:HA	2:B:149:ALA:O	2.20	0.42
1:E:135:GLY:C	1:E:137:ASN:N	2.77	0.42
2:F:30:ILE:O	2:F:32:ALA:N	2.52	0.42
1:G:119:PRO:HB3	1:G:173:GLY:O	2.20	0.42
1:A:51:ARG:O	1:A:52:GLU:C	2.62	0.42
2:D:4:LEU:HD21	2:D:99:LEU:HD22	2.00	0.42
2:F:33:THR:O	2:F:73:ARG:NH2	2.53	0.42
2:B:53:SER:HB2	2:B:55:ASP:OD2	2.20	0.41
2:B:209:ARG:NH1	2:B:209:ARG:HG2	2.35	0.41
1:C:53:LYS:O	1:C:55:ILE:HG13	2.20	0.41
2:D:99:LEU:HD23	2:D:99:LEU:C	2.45	0.41
1:E:119:PRO:HD2	1:E:175:TYR:CZ	2.54	0.41
1:G:72:LYS:O	1:G:73:ASN:C	2.63	0.41
2:H:12:THR:O	2:H:13:LYS:HD3	2.20	0.41
2:F:144:THR:HA	2:F:149:ALA:O	2.20	0.41
1:G:135:GLY:C	1:G:137:ASN:N	2.77	0.41
1:G:150:ILE:HD11	1:G:193:VAL:CG1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:LEU:O	2:F:16:SER:HB2	2.19	0.41
1:G:69:ASP:C	1:G:71:ALA:N	2.78	0.41
1:A:29:ALA:HB3	1:A:32:ASN:ND2	2.35	0.41
2:B:170:GLU:O	2:B:171:LYS:C	2.63	0.41
2:B:213:ARG:HE	2:B:222:ASP:CG	2.28	0.41
2:F:34:SER:OG	2:F:53:SER:HA	2.21	0.41
2:H:145:LYS:HD2	2:H:145:LYS:N	2.35	0.41
2:B:41:ARG:HG3	2:B:42:PRO:HD2	2.03	0.41
1:C:2:ILE:HD13	1:C:108:ILE:HD12	2.02	0.41
2:F:77:THR:OG1	2:F:79:THR:HG22	2.20	0.41
2:F:139:PRO:HG3	2:F:151:THR:C	2.45	0.41
2:B:61:GLU:HG3	2:B:62:SER:N	2.34	0.41
1:A:72:LYS:O	1:A:73:ASN:C	2.63	0.41
2:B:31:SER:O	2:B:32:ALA:CB	2.68	0.41
1:C:126:LYS:HE3	1:C:200:VAL:HG22	2.01	0.41
1:C:167:ILE:N	1:C:167:ILE:HD12	2.36	0.41
2:D:5:GLU:HB2	2:D:24:VAL:CG2	2.46	0.41
2:D:87:VAL:CG2	2:D:121:ILE:HD11	2.49	0.41
2:D:177:LEU:HD22	2:D:197:LEU:HD21	2.02	0.41
1:E:69:ASP:OD1	1:E:71:ALA:HB3	2.21	0.41
1:E:87:GLU:HG3	1:E:115:VAL:O	2.21	0.41
1:E:126:LYS:HE3	1:E:200:VAL:HG22	2.03	0.41
2:F:72:ASP:OD1	2:F:72:ASP:C	2.64	0.41
2:F:171:LYS:HD3	2:F:209:ARG:HH22	1.86	0.41
2:H:177:LEU:HD22	2:H:197:LEU:HD21	2.02	0.41
2:B:4:LEU:HD21	2:B:99:LEU:HD22	2.03	0.41
2:B:17:LYS:HD2	2:B:17:LYS:HA	1.85	0.41
2:D:145:LYS:HD2	2:D:145:LYS:N	2.36	0.41
1:G:132:MET:H	1:G:132:MET:HG2	1.64	0.41
1:A:67:ASP:O	1:A:76:VAL:HG22	2.21	0.40
1:C:25:MET:HG2	1:C:26:LYS:N	2.36	0.40
1:C:145:PHE:O	1:C:175:TYR:HB2	2.21	0.40
2:D:15:LEU:H	2:D:15:LEU:CD1	2.29	0.40
1:A:25:MET:HE3	1:A:30:ILE:HD12	2.03	0.40
1:A:203:THR:C	1:A:205:PHE:H	2.28	0.40
2:D:168:TRP:O	2:D:169:GLU:HG3	2.21	0.40
1:C:36:ASN:ND2	1:C:51:ARG:HG3	2.37	0.40
1:C:55:ILE:CG1	2:D:108:LYS:HE3	2.51	0.40
1:E:146:TYR:CG	1:E:147:PRO:HA	2.55	0.40
1:G:36:ASN:HA	1:G:50:TYR:O	2.21	0.40
2:H:214:HIS:H	2:H:217:ASN:ND2	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:NE2	1:A:174:LYS:HE2	2.36	0.40
1:E:136:THR:HA	1:E:183:TYR:O	2.21	0.40
2:F:137:PHE:HB2	2:F:153:LEU:HB3	2.04	0.40
2:D:24:VAL:O	2:D:24:VAL:CG2	2.69	0.40
2:D:27:GLY:O	2:D:28:ILE:HD13	2.21	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	204/229 (89%)	178 (87%)	19 (9%)	7 (3%)	3	15
1	C	204/229 (89%)	184 (90%)	16 (8%)	4 (2%)	6	24
1	E	204/229 (89%)	180 (88%)	18 (9%)	6 (3%)	3	18
1	G	204/229 (89%)	179 (88%)	17 (8%)	8 (4%)	2	13
2	B	228/242 (94%)	191 (84%)	33 (14%)	4 (2%)	6	26
2	D	228/242 (94%)	199 (87%)	25 (11%)	4 (2%)	6	26
2	F	228/242 (94%)	199 (87%)	22 (10%)	7 (3%)	3	17
2	H	228/242 (94%)	188 (82%)	29 (13%)	11 (5%)	2	10
All	All	1728/1884 (92%)	1498 (87%)	179 (10%)	51 (3%)	3	17

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	32	ALA
2	D	171	LYS
2	F	30	ILE
2	F	31	SER
2	F	171	LYS

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Mol	Chain	Res	Type
2	H	30	ILE
2	H	32	ALA
2	H	171	LYS
2	H	174	ASN
1	A	27	GLY
1	A	52	GLU
1	A	54	ASP
1	A	135	GLY
2	B	229	PRO
1	C	135	GLY
2	D	32	ALA
2	D	229	PRO
1	E	73	ASN
1	E	135	GLY
2	F	229	PRO
1	G	100	GLY
1	G	135	GLY
2	H	31	SER
2	H	229	PRO
1	A	134	ASN
1	C	52	GLU
1	E	54	ASP
1	E	134	ASN
2	F	126	LEU
2	F	174	ASN
2	H	55	ASP
1	A	144	GLU
2	B	31	SER
1	C	134	ASN
2	D	146	LEU
1	E	53	LYS
1	E	144	GLU
2	F	146	LEU
1	G	52	GLU
1	G	103	TYR
1	G	134	ASN
1	G	144	GLU
2	B	146	LEU
1	C	144	GLU
1	G	98	GLY
2	H	78	SER
2	H	103	GLN

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Mol	Chain	Res	Type
2	H	146	LEU
1	A	103	TYR
1	G	70	ILE
2	H	161	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	180/203 (89%)	172 (96%)	8 (4%)	25	54
1	C	180/203 (89%)	168 (93%)	12 (7%)	15	41
1	E	180/203 (89%)	170 (94%)	10 (6%)	19	47
1	G	180/203 (89%)	168 (93%)	12 (7%)	15	41
2	B	208/220 (94%)	194 (93%)	14 (7%)	15	41
2	D	208/220 (94%)	193 (93%)	15 (7%)	13	39
2	F	208/220 (94%)	191 (92%)	17 (8%)	10	34
2	H	208/220 (94%)	190 (91%)	18 (9%)	9	32
All	All	1552/1692 (92%)	1446 (93%)	106 (7%)	14	40

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	74	LEU
1	A	92	CYS
1	A	97	LEU
1	A	103	TYR
1	A	113	THR
1	A	131	VAL
1	A	132	MET
2	B	18	THR
2	B	21	LEU
2	B	25	VAL

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Mol	Chain	Res	Type
2	B	30	ILE
2	B	41	ARG
2	B	71	VAL
2	B	73	ARG
2	B	79	THR
2	B	99	LEU
2	B	130	VAL
2	B	145	LYS
2	B	153	LEU
2	B	162	ASP
2	B	192	MET
1	C	2	ILE
1	C	35	ILE
1	C	42	GLN
1	C	92	CYS
1	C	102	GLU
1	C	103	TYR
1	C	113	THR
1	C	115	VAL
1	C	128	SER
1	C	131	VAL
1	C	132	MET
1	C	158	LYS
2	D	18	THR
2	D	21	LEU
2	D	25	VAL
2	D	30	ILE
2	D	33	THR
2	D	41	ARG
2	D	71	VAL
2	D	79	THR
2	D	99	LEU
2	D	130	VAL
2	D	134	PRO
2	D	145	LYS
2	D	153	LEU
2	D	162	ASP
2	D	192	MET
1	E	2	ILE
1	E	74	LEU
1	E	92	CYS
1	E	97	LEU

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Mol	Chain	Res	Type
1	E	102	GLU
1	E	103	TYR
1	E	113	THR
1	E	120	ARG
1	E	131	VAL
1	E	132	MET
2	F	18	THR
2	F	21	LEU
2	F	25	VAL
2	F	29	THR
2	F	30	ILE
2	F	41	ARG
2	F	71	VAL
2	F	73	ARG
2	F	99	LEU
2	F	104	GLN
2	F	123	ASP
2	F	130	VAL
2	F	134	PRO
2	F	145	LYS
2	F	153	LEU
2	F	162	ASP
2	F	192	MET
1	G	2	ILE
1	G	35	ILE
1	G	42	GLN
1	G	70	ILE
1	G	72	LYS
1	G	74	LEU
1	G	92	CYS
1	G	97	LEU
1	G	113	THR
1	G	131	VAL
1	G	132	MET
1	G	158	LYS
2	H	18	THR
2	H	21	LEU
2	H	25	VAL
2	H	30	ILE
2	H	33	THR
2	H	41	ARG
2	H	54	TYR

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Mol	Chain	Res	Type
2	H	71	VAL
2	H	78	SER
2	H	99	LEU
2	H	104	GLN
2	H	110	ILE
2	H	126	LEU
2	H	130	VAL
2	H	145	LYS
2	H	153	LEU
2	H	162	ASP
2	H	192	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	32	ASN
1	A	36	ASN
1	A	42	GLN
1	A	122	GLN
1	A	137	ASN
1	A	194	GLN
2	B	3	HIS
2	B	90	GLN
2	B	147	GLN
2	B	180	GLN
2	B	214	HIS
2	B	216	ASN
2	B	223	GLN
1	C	8	HIS
1	C	32	ASN
1	C	36	ASN
1	C	42	GLN
1	C	73	ASN
1	C	122	GLN
1	C	137	ASN
1	C	194	GLN
2	D	3	HIS
2	D	90	GLN
2	D	216	ASN
2	D	223	GLN
1	E	8	HIS

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Mol	Chain	Res	Type
1	E	36	ASN
1	E	122	GLN
1	E	137	ASN
1	E	153	ASN
2	F	3	HIS
2	F	90	GLN
2	F	103	GLN
2	F	180	GLN
2	F	208	HIS
2	F	214	HIS
2	F	223	GLN
1	G	8	HIS
1	G	9	GLN
1	G	36	ASN
1	G	122	GLN
1	G	137	ASN
1	G	153	ASN
1	G	195	HIS
2	H	90	GLN
2	H	167	HIS
2	H	214	HIS
2	H	217	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	D	1002	-	4,4,4	0.28	0	6,6,6	0.17	0
3	SO4	F	1001	-	4,4,4	0.38	0	6,6,6	0.19	0

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

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.