



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:24 AM UTC

PDB ID : 7YA2 / pdb_00007ya2
Title : Crystal structure of capsular polysaccharide synthesis enzyme CapG from *Staphylococcus aureus*
Authors : Chen, Y.; Wang, Y.C.
Deposited on : 2022-06-27
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

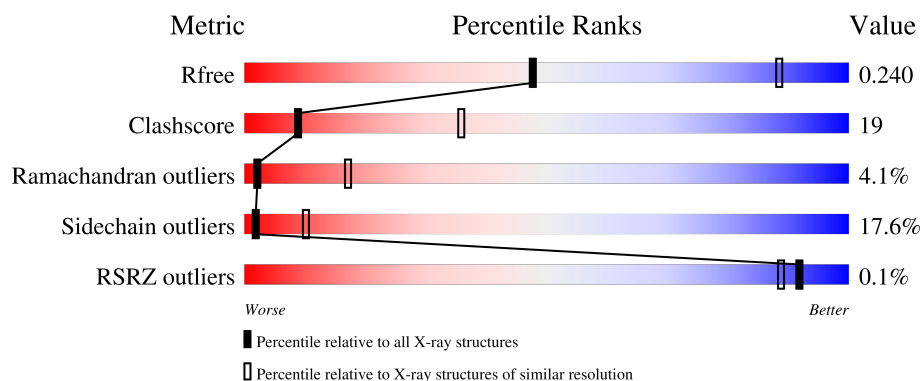
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

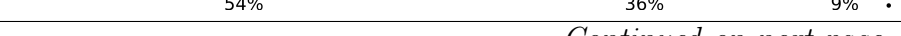
The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	374	 61% 26% 11% ..
1	B	374	 59% 30% 9% .
1	C	374	 56% 35% 7% .
1	D	374	 52% 36% 10% .
1	E	374	 54% 36% 9% .

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Mol	Chain	Length	Quality of chain
1	F	374	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: green (52%), yellow (37%), and red (9%). A small black dot is at the end of the red segment.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18050 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.

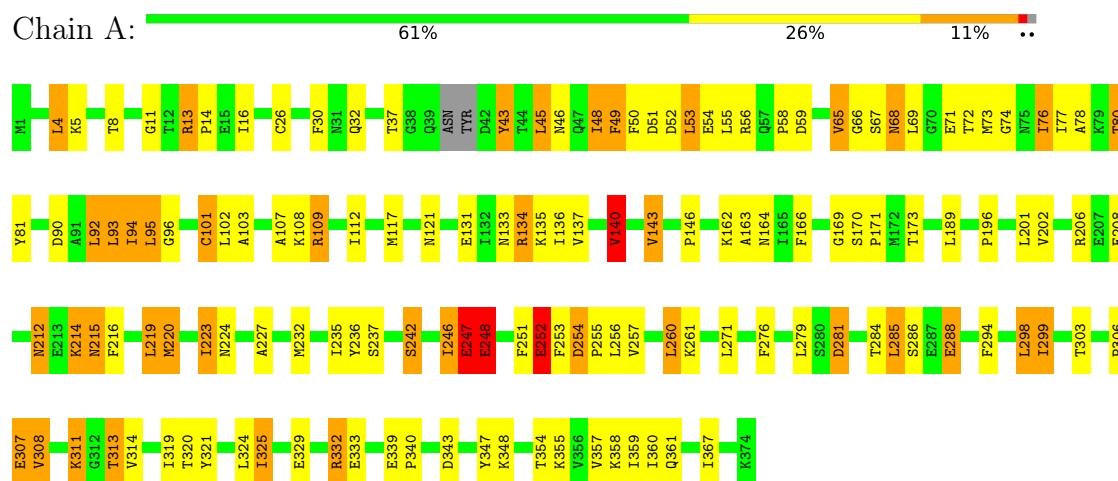
- Molecule 1 is a protein called Capsular polysaccharide synthesis enzyme CapG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2995	1898	512	573	12			
1	B	374	Total	C	N	O	S	0	0	0
			3011	1909	513	577	12			
1	C	374	Total	C	N	O	S	0	0	0
			3011	1909	513	577	12			
1	D	374	Total	C	N	O	S	0	0	0
			3011	1909	513	577	12			
1	E	374	Total	C	N	O	S	0	0	0
			3011	1909	513	577	12			
1	F	374	Total	C	N	O	S	0	0	0
			3011	1909	513	577	12			

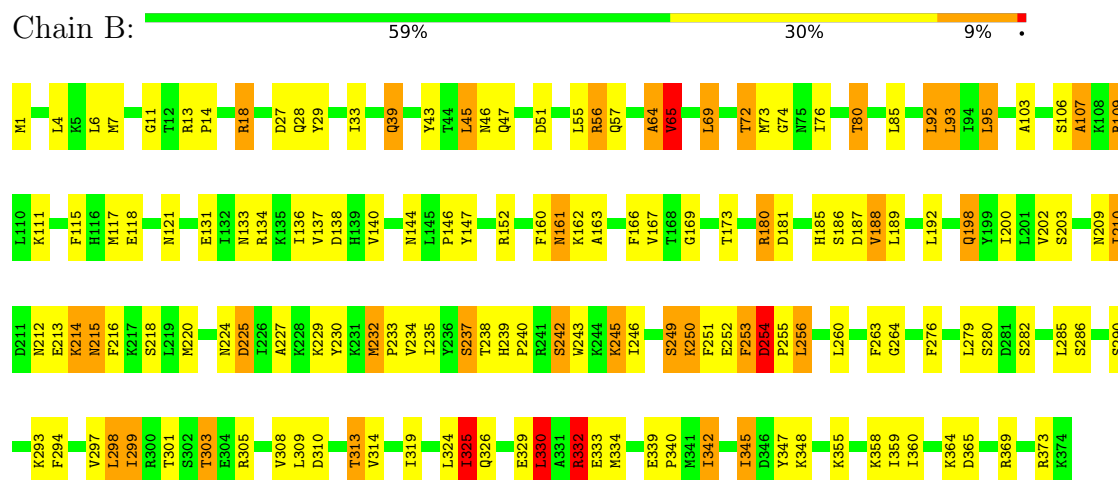
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Capsular polysaccharide synthesis enzyme CapG

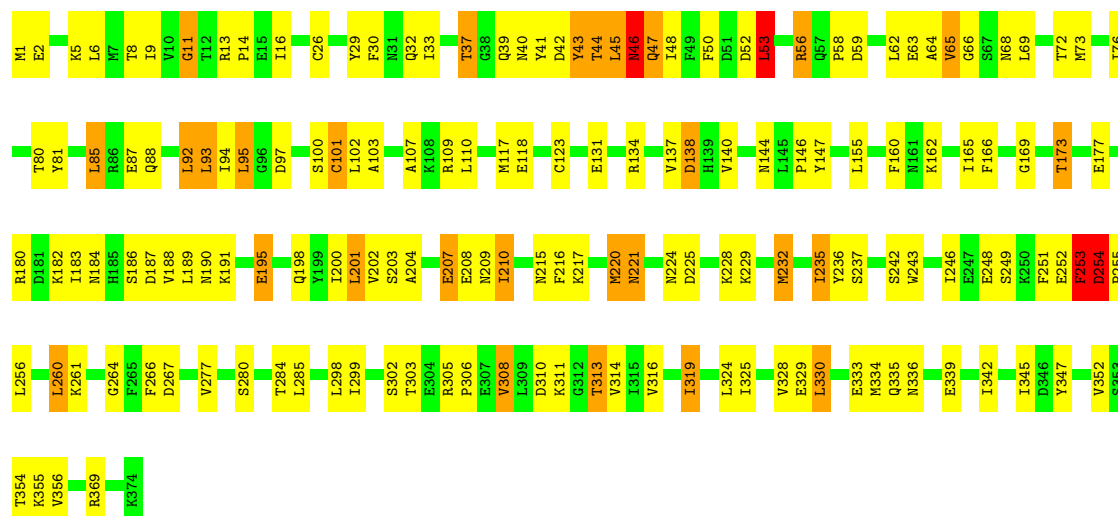


- Molecule 1: Capsular polysaccharide synthesis enzyme CapG



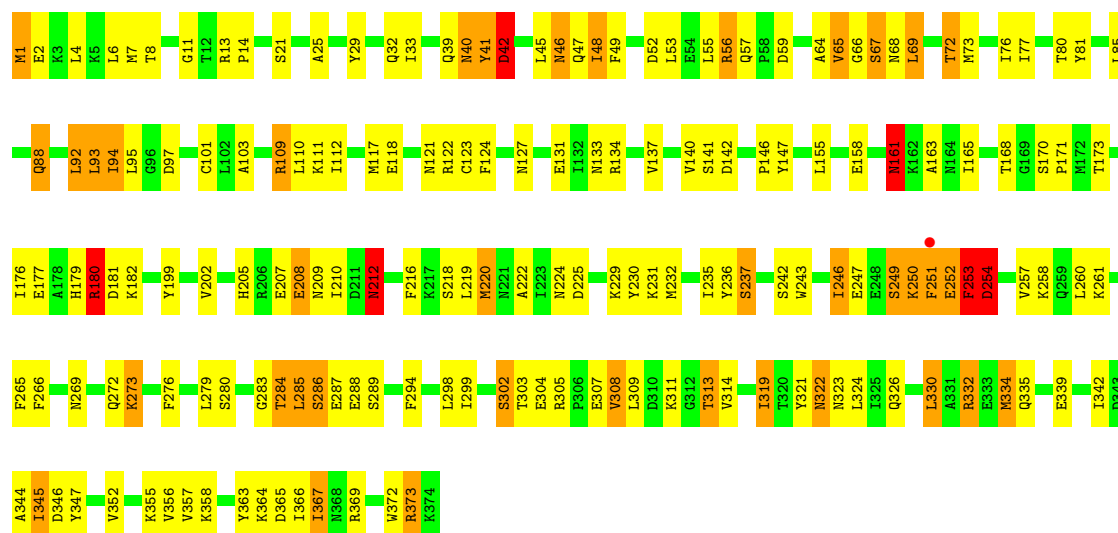
- Molecule 1: Capsular polysaccharide synthesis enzyme CapG





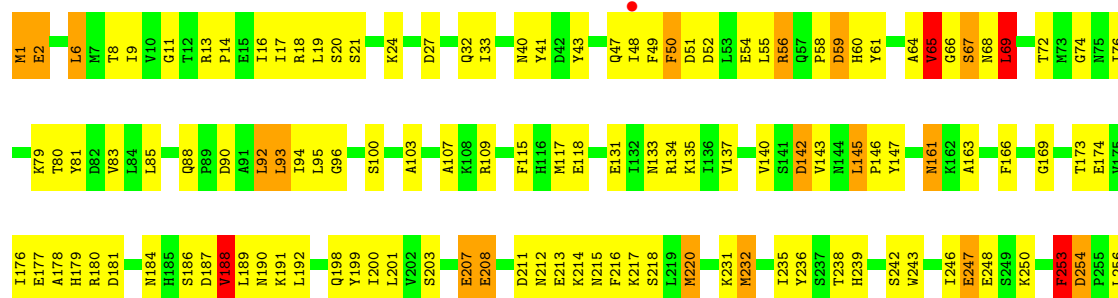
• Molecule 1: Capsular polysaccharide synthesis enzyme CapG

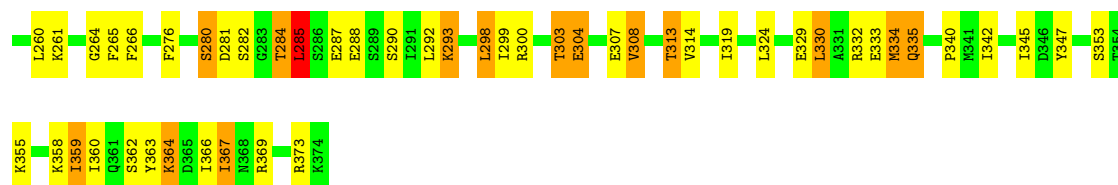
Chain D: 52% 36% 10%



• Molecule 1: Capsular polysaccharide synthesis enzyme CapG

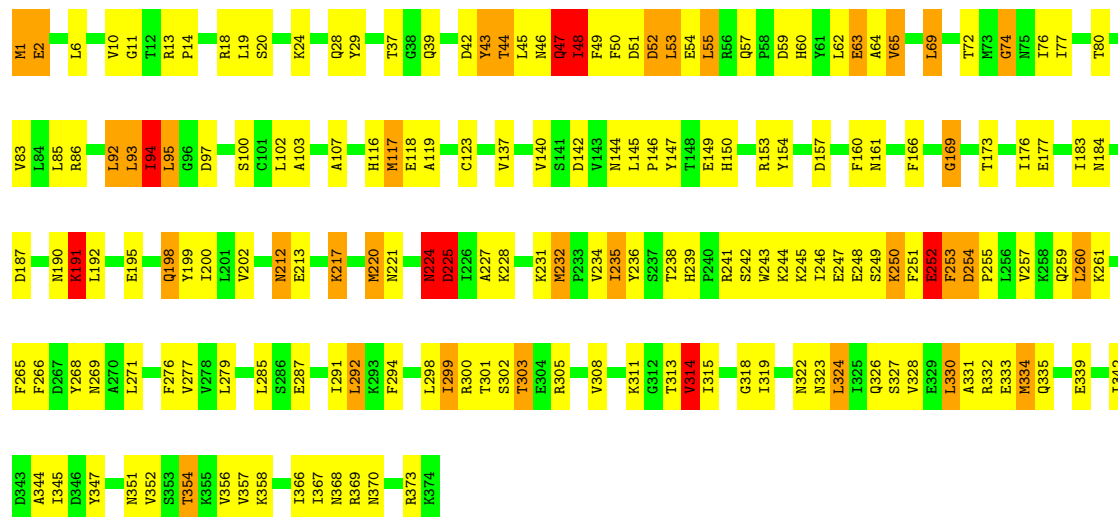
Chain E: 54% 36% 9%





- Molecule 1: Capsular polysaccharide synthesis enzyme CapG

Chain F: 52% 37% 9% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	302.91Å 84.34Å 145.09Å 90.00° 110.65° 90.00°	Depositor
Resolution (Å)	25.57 – 3.20 25.57 – 3.20	Depositor EDS
% Data completeness (in resolution range)	87.9 (25.57-3.20) 87.9 (25.57-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.17Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.183 , 0.241 0.185 , 0.240	Depositor DCC
R_{free} test set	2558 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18050	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	1.05	1/3049 (0.0%)	1.50	8/4122 (0.2%)
1	B	1.06	0/3066	1.49	9/4146 (0.2%)
1	C	1.06	0/3066	1.49	5/4146 (0.1%)
1	D	1.06	1/3066 (0.0%)	1.47	9/4146 (0.2%)
1	E	1.05	1/3066 (0.0%)	1.49	2/4146 (0.0%)
1	F	1.04	0/3066	1.48	4/4146 (0.1%)
All	All	1.05	3/18379 (0.0%)	1.49	37/24852 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	E	0	3
1	F	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	340	PRO	C-O	-5.89	1.17	1.23
1	D	112	ILE	N-CA	5.26	1.50	1.46
1	A	112	ILE	N-CA	5.10	1.50	1.46

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	169	GLY	CA-C-O	-8.08	115.13	122.57
1	D	253	PHE	CA-CB-CG	7.70	121.50	113.80
1	C	169	GLY	CA-C-O	-6.90	116.22	122.57
1	E	169	GLY	CA-C-O	-6.79	117.15	122.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	PHE	CA-CB-CG	6.42	120.22	113.80
1	B	111	LYS	CA-C-N	6.07	126.96	122.59
1	B	111	LYS	C-N-CA	6.07	126.96	122.59
1	B	169	GLY	CA-C-O	-5.84	116.96	122.39
1	A	281	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	355	LYS	CA-C-N	5.64	127.78	120.56
1	A	355	LYS	C-N-CA	5.64	127.78	120.56
1	F	102	LEU	N-CA-C	-5.61	106.52	113.19
1	A	169	GLY	CA-C-O	-5.47	117.30	122.39
1	D	73	MET	CA-C-N	5.33	125.99	120.03
1	D	73	MET	C-N-CA	5.33	125.99	120.03
1	B	310	ASP	CA-CB-CG	5.32	117.92	112.60
1	F	225	ASP	CA-C-N	5.24	127.11	120.72
1	F	225	ASP	C-N-CA	5.24	127.11	120.72
1	E	140	VAL	N-CA-C	-5.19	108.23	113.47
1	D	283	GLY	CA-C-N	5.16	128.56	120.82
1	D	283	GLY	C-N-CA	5.16	128.56	120.82
1	B	162	LYS	CA-C-N	5.15	127.18	120.28
1	B	162	LYS	C-N-CA	5.15	127.18	120.28
1	A	102	LEU	N-CA-C	-5.15	106.83	113.01
1	B	313	THR	N-CA-C	-5.14	108.04	114.56
1	A	355	LYS	O-C-N	5.13	127.56	122.12
1	A	66	GLY	CA-C-O	-5.10	118.20	122.33
1	C	102	LEU	N-CA-C	-5.08	107.03	113.18
1	C	44	THR	CA-C-N	5.07	127.84	120.79
1	C	44	THR	C-N-CA	5.07	127.84	120.79
1	D	161	ASN	CA-C-N	5.06	127.32	120.38
1	D	161	ASN	C-N-CA	5.06	127.32	120.38
1	A	49	PHE	CA-C-O	-5.06	116.19	121.55
1	D	283	GLY	O-C-N	5.04	127.06	122.17
1	D	88	GLN	CB-CA-C	5.03	114.77	111.20
1	B	332	ARG	N-CA-C	-5.03	105.49	110.97
1	B	138	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	ASN	Peptide
1	A	96	GLY	Peptide
1	E	253	PHE	Peptide
1	E	41	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	E	50	PHE	Peptide
1	F	52	ASP	Peptide

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	2995	0	3006	112	0
1	B	3011	0	3013	108	0
1	C	3011	0	3013	107	0
1	D	3011	0	3013	132	0
1	E	3011	0	3013	119	0
1	F	3011	0	3013	132	0
All	All	18050	0	18071	671	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 19.

All (671) 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)
1:C:173:THR:HG21	1:C:347:TYR:O	1.46	1.13
1:B:95:LEU:HD22	1:B:117:MET:HB3	1.45	0.99
1:A:219:LEU:CD2	1:A:299:ILE:HD11	1.95	0.96
1:A:219:LEU:HD21	1:A:299:ILE:HD11	1.48	0.96
1:C:64:ALA:O	1:C:65:VAL:HG12	1.65	0.95
1:E:76:ILE:O	1:E:80:THR:OG1	1.84	0.93
1:A:235:ILE:HG23	1:A:260:LEU:HG	1.50	0.93
1:A:215:ASN:HD22	1:A:319:ILE:HD13	1.36	0.91
1:B:133:ASN:O	1:B:137:VAL:HG12	1.72	0.90
1:D:173:THR:HG21	1:D:347:TYR:O	1.72	0.90
1:F:173:THR:HG21	1:F:347:TYR:O	1.71	0.89
1:A:242:SER:O	1:A:246:ILE:CG2	2.21	0.89
1:A:219:LEU:HD21	1:A:299:ILE:CD1	2.03	0.88
1:B:46:ASN:HD21	1:B:57:GLN:HE22	1.20	0.87
1:D:358:LYS:HE3	1:F:334:MET:HE3	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ILE:HG22	1:C:260:LEU:HG	1.57	0.86
1:A:242:SER:O	1:A:246:ILE:HG23	1.74	0.85
1:A:339:GLU:OE2	1:C:29:TYR:OH	1.96	0.84
1:E:173:THR:HG21	1:E:347:TYR:O	1.78	0.83
1:C:330:LEU:HD22	1:C:334:MET:HE2	1.59	0.82
1:B:146:PRO:HD2	1:B:166:PHE:O	1.80	0.81
1:C:201:LEU:HD12	1:C:202:VAL:N	1.96	0.80
1:C:243:TRP:O	1:C:246:ILE:HG22	1.80	0.80
1:A:358:LYS:HE3	1:E:334:MET:HE3	1.65	0.79
1:D:56:ARG:NH1	1:D:59:ASP:OD1	2.16	0.79
1:A:76:ILE:O	1:A:80:THR:HB	1.83	0.79
1:B:95:LEU:CD2	1:B:117:MET:HB3	2.13	0.78
1:B:173:THR:HG21	1:B:347:TYR:O	1.82	0.78
1:C:80:THR:HG21	1:C:103:ALA:HA	1.62	0.78
1:A:215:ASN:HD22	1:A:319:ILE:CD1	1.96	0.78
1:D:76:ILE:O	1:D:80:THR:OG1	2.01	0.77
1:A:80:THR:HG21	1:A:103:ALA:HA	1.65	0.77
1:F:277:VAL:HG11	1:F:328:VAL:HG13	1.68	0.76
1:F:95:LEU:HD22	1:F:117:MET:HB3	1.68	0.76
1:A:143:VAL:HG23	1:A:367:ILE:HD11	1.68	0.75
1:F:92:LEU:HD22	1:F:93:LEU:O	1.85	0.75
1:B:235:ILE:HG22	1:B:260:LEU:HG	1.68	0.75
1:B:358:LYS:HE2	1:D:334:MET:HE3	1.67	0.75
1:C:195:GLU:HB2	1:C:198:GLN:HG3	1.67	0.75
1:E:304:GLU:N	1:E:304:GLU:OE1	2.20	0.75
1:E:8:THR:OG1	1:E:32:GLN:NE2	2.20	0.74
1:F:254:ASP:OD1	1:F:255:PRO:HD2	1.87	0.74
1:A:253:PHE:O	1:A:254:ASP:O	2.05	0.74
1:D:179:HIS:O	1:D:182:LYS:N	2.19	0.74
1:F:368:ASN:O	1:F:373:ARG:N	2.21	0.74
1:C:187:ASP:O	1:C:189:LEU:N	2.19	0.74
1:B:76:ILE:O	1:B:80:THR:OG1	2.06	0.74
1:E:6:LEU:HD21	1:E:93:LEU:HB2	1.69	0.73
1:F:334:MET:HG3	1:F:339:GLU:HG3	1.68	0.73
1:A:220:MET:HE1	1:A:236:TYR:OH	1.89	0.73
1:F:212:ASN:C	1:F:212:ASN:HD22	1.97	0.73
1:F:80:THR:HG21	1:F:103:ALA:HA	1.71	0.73
1:E:58:PRO:HG2	1:E:61:TYR:CE2	2.23	0.73
1:E:186:SER:OG	1:E:188:VAL:HG12	1.89	0.73
1:A:50:PHE:O	1:A:54:GLU:HA	1.87	0.73
1:B:43:TYR:O	1:B:47:GLN:HB2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:SER:C	1:D:246:ILE:HG23	2.15	0.72
1:C:228:LYS:HG2	1:C:254:ASP:OD2	1.90	0.71
1:F:45:LEU:O	1:F:48:ILE:HG12	1.90	0.71
1:D:344:ALA:HB3	1:D:347:TYR:CD2	2.25	0.71
1:F:332:ARG:HG3	1:F:333:GLU:N	2.04	0.71
1:D:242:SER:O	1:D:246:ILE:HG23	1.91	0.70
1:A:254:ASP:CG	1:A:255:PRO:HD2	2.16	0.70
1:D:133:ASN:O	1:D:137:VAL:HG12	1.92	0.70
1:C:56:ARG:NH1	1:C:59:ASP:OD1	2.25	0.70
1:D:137:VAL:O	1:D:141:SER:OG	2.08	0.69
1:E:69:LEU:HA	1:E:72:THR:CG2	2.23	0.69
1:B:242:SER:C	1:B:246:ILE:HG23	2.18	0.69
1:A:4:LEU:HD12	1:A:5:LYS:N	2.07	0.69
1:F:224:ASN:HD21	1:F:253:PHE:HA	1.58	0.69
1:B:358:LYS:CE	1:D:334:MET:HE3	2.21	0.69
1:C:146:PRO:HD2	1:C:166:PHE:O	1.93	0.69
1:D:322:ASN:C	1:D:322:ASN:HD22	2.01	0.69
1:E:284:THR:O	1:E:287:GLU:N	2.25	0.69
1:F:18:ARG:NH1	1:F:118:GLU:OE1	2.26	0.68
1:A:173:THR:HG21	1:A:347:TYR:O	1.93	0.68
1:A:299:ILE:HG12	1:A:299:ILE:O	1.93	0.68
1:C:235:ILE:CG2	1:C:260:LEU:HG	2.24	0.68
1:D:179:HIS:O	1:D:181:ASP:N	2.27	0.67
1:D:220:MET:HE1	1:D:236:TYR:OH	1.93	0.67
1:D:8:THR:OG1	1:D:32:GLN:NE2	2.27	0.67
1:E:13:ARG:HD3	1:E:50:PHE:CE2	2.30	0.67
1:B:243:TRP:HA	1:B:246:ILE:HG12	1.75	0.66
1:B:65:VAL:HA	1:B:72:THR:HB	1.77	0.66
1:A:311:LYS:HA	1:C:355:LYS:HE2	1.77	0.66
1:D:355:LYS:HE2	1:F:311:LYS:HA	1.77	0.66
1:E:187:ASP:O	1:E:190:ASN:N	2.29	0.66
1:A:339:GLU:HG3	1:A:340:PRO:HD2	1.79	0.65
1:B:95:LEU:HD22	1:B:117:MET:CB	2.24	0.65
1:F:200:ILE:HG13	1:F:232:MET:HE2	1.79	0.65
1:C:80:THR:HG21	1:C:103:ALA:CA	2.27	0.64
1:F:313:THR:O	1:F:313:THR:HG22	1.97	0.64
1:A:95:LEU:CD2	1:A:117:MET:HB3	2.28	0.64
1:A:219:LEU:CD2	1:A:299:ILE:CD1	2.68	0.64
1:E:118:GLU:HG3	1:E:147:TYR:CE2	2.33	0.63
1:A:361:GLN:HG3	1:E:330:LEU:HD12	1.80	0.63
1:B:39:GLN:HE21	1:B:39:GLN:C	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ASP:HB3	1:D:367:ILE:HD12	1.81	0.63
1:D:6:LEU:HD23	1:D:7:MET:N	2.14	0.62
1:E:178:ALA:O	1:E:179:HIS:ND1	2.31	0.62
1:F:142:ASP:HB3	1:F:367:ILE:HD12	1.81	0.62
1:A:219:LEU:HD23	1:A:299:ILE:HD11	1.82	0.62
1:A:232:MET:C	1:A:256:LEU:HD23	2.23	0.62
1:D:224:ASN:ND2	1:D:253:PHE:HB2	2.14	0.62
1:D:289:SER:HB3	1:D:294:PHE:CE1	2.35	0.62
1:E:253:PHE:O	1:E:254:ASP:O	2.18	0.61
1:D:92:LEU:HD23	1:D:93:LEU:N	2.15	0.61
1:B:332:ARG:HG3	1:B:333:GLU:N	2.15	0.61
1:F:123:CYS:HB2	1:F:302:SER:HB2	1.83	0.61
1:D:64:ALA:O	1:D:65:VAL:HB	2.00	0.61
1:C:94:ILE:HG23	1:C:101:CYS:HB3	1.82	0.60
1:B:242:SER:O	1:B:246:ILE:HG23	2.02	0.60
1:C:311:LYS:HA	1:E:355:LYS:HE2	1.83	0.60
1:E:95:LEU:HD22	1:E:117:MET:HB3	1.82	0.60
1:F:212:ASN:HD22	1:F:213:GLU:N	1.99	0.60
1:D:146:PRO:HG3	1:D:155:LEU:HD12	1.83	0.60
1:D:81:TYR:CZ	1:D:110:LEU:HD21	2.37	0.60
1:E:131:GLU:HA	1:E:134:ARG:HD2	1.82	0.60
1:A:212:ASN:HB3	1:A:215:ASN:OD1	2.01	0.60
1:B:212:ASN:HB3	1:B:215:ASN:HD22	1.66	0.60
1:C:201:LEU:HD12	1:C:202:VAL:H	1.67	0.60
1:E:363:TYR:O	1:E:367:ILE:HG13	2.01	0.59
1:F:69:LEU:HA	1:F:72:THR:CG2	2.32	0.59
1:B:330:LEU:HD22	1:B:334:MET:HE2	1.83	0.59
1:D:6:LEU:HD21	1:D:93:LEU:HB2	1.84	0.59
1:C:173:THR:CG2	1:C:347:TYR:O	2.38	0.59
1:E:90:ASP:HB3	1:E:364:LYS:HE2	1.83	0.59
1:E:254:ASP:HB3	1:E:256:LEU:HD12	1.85	0.59
1:A:358:LYS:CE	1:E:334:MET:CE	2.81	0.59
1:B:64:ALA:O	1:B:65:VAL:HB	2.01	0.59
1:B:249:SER:OG	1:B:250:LYS:N	2.36	0.59
1:E:199:TYR:N	1:E:232:MET:HE3	2.18	0.59
1:E:220:MET:HE1	1:E:236:TYR:OH	2.01	0.59
1:C:40:ASN:O	1:C:43:TYR:N	2.30	0.58
1:C:308:VAL:HG13	1:C:313:THR:HG22	1.85	0.58
1:A:92:LEU:HD12	1:A:107:ALA:HB2	1.84	0.58
1:A:146:PRO:HD2	1:A:166:PHE:O	2.02	0.58
1:E:85:LEU:O	1:E:88:GLN:HG2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ASN:CG	1:C:319:ILE:HG21	2.28	0.58
1:E:56:ARG:HD3	1:E:56:ARG:C	2.29	0.58
1:E:64:ALA:O	1:E:65:VAL:HB	2.03	0.58
1:A:68:ASN:ND2	1:A:71:GLU:H	2.02	0.58
1:B:152:ARG:NH2	1:B:167:VAL:HG23	2.19	0.57
1:F:199:TYR:OH	1:F:271:LEU:O	2.22	0.57
1:D:199:TYR:N	1:D:232:MET:HE3	2.19	0.57
1:C:94:ILE:CG2	1:C:101:CYS:HB3	2.35	0.57
1:A:298:LEU:HD22	1:A:298:LEU:C	2.30	0.57
1:E:68:ASN:O	1:E:72:THR:HG22	2.05	0.57
1:D:45:LEU:HA	1:D:48:ILE:CG2	2.35	0.57
1:E:51:ASP:O	1:E:54:GLU:N	2.37	0.57
1:E:1:MET:HG2	1:E:2:GLU:H	1.70	0.56
1:D:276:PHE:CZ	1:D:332:ARG:HB2	2.40	0.56
1:A:4:LEU:HD12	1:A:4:LEU:C	2.31	0.56
1:A:254:ASP:OD2	1:A:255:PRO:HD2	2.05	0.56
1:B:118:GLU:HG3	1:B:147:TYR:CE2	2.41	0.56
1:D:173:THR:CG2	1:D:347:TYR:O	2.52	0.56
1:F:352:VAL:O	1:F:356:VAL:HG23	2.05	0.56
1:A:284:THR:O	1:A:288:GLU:CG	2.53	0.56
1:C:45:LEU:C	1:C:47:GLN:H	2.12	0.56
1:B:235:ILE:CG2	1:B:260:LEU:HG	2.36	0.56
1:F:217:LYS:O	1:F:221:ASN:HB2	2.06	0.56
1:A:202:VAL:HG11	1:A:223:ILE:HD11	1.88	0.56
1:E:329:GLU:O	1:E:333:GLU:HB2	2.05	0.56
1:C:334:MET:HG3	1:C:339:GLU:HG3	1.88	0.56
1:F:323:ASN:O	1:F:326:GLN:N	2.38	0.56
1:B:276:PHE:CZ	1:B:332:ARG:HB2	2.40	0.55
1:F:199:TYR:CA	1:F:232:MET:HE3	2.36	0.55
1:A:131:GLU:HA	1:A:134:ARG:HD2	1.88	0.55
1:D:216:PHE:HZ	1:D:246:ILE:HG22	1.71	0.55
1:A:358:LYS:CE	1:E:334:MET:HE3	2.36	0.55
1:C:80:THR:HG21	1:C:103:ALA:CB	2.36	0.55
1:F:199:TYR:HA	1:F:232:MET:HE3	1.89	0.55
1:D:334:MET:HG3	1:D:339:GLU:HG3	1.87	0.55
1:A:95:LEU:HD22	1:A:117:MET:HB3	1.88	0.55
1:B:161:ASN:C	1:B:161:ASN:HD22	2.15	0.55
1:A:235:ILE:CG2	1:A:260:LEU:HG	2.30	0.54
1:A:56:ARG:NH1	1:A:59:ASP:OD2	2.39	0.54
1:C:5:LYS:NZ	1:C:87:GLU:O	2.40	0.54
1:D:237:SER:HB2	1:D:260:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ASP:O	1:C:53:LEU:HB2	2.06	0.54
1:F:92:LEU:HD12	1:F:107:ALA:CB	2.38	0.54
1:D:253:PHE:O	1:D:254:ASP:O	2.24	0.54
1:E:80:THR:HG21	1:E:103:ALA:CB	2.38	0.54
1:C:11:GLY:HA3	1:C:100:SER:OG	2.07	0.54
1:A:68:ASN:ND2	1:A:68:ASN:O	2.37	0.54
1:A:321:TYR:CZ	1:A:325:ILE:HD11	2.43	0.54
1:F:137:VAL:HA	1:F:140:VAL:CG1	2.37	0.54
1:C:203:SER:O	1:C:280:SER:HA	2.07	0.53
1:E:49:PHE:HB3	1:E:50:PHE:HD2	1.71	0.53
1:F:10:VAL:HG12	1:F:19:LEU:HD12	1.90	0.53
1:A:163:ALA:C	1:A:164:ASN:HD22	2.17	0.53
1:A:253:PHE:C	1:A:254:ASP:O	2.50	0.53
1:B:237:SER:CB	1:B:260:LEU:HD12	2.38	0.53
1:D:118:GLU:HG3	1:D:147:TYR:CE2	2.43	0.53
1:E:18:ARG:NH1	1:E:118:GLU:OE1	2.41	0.53
1:E:81:TYR:CZ	1:F:69:LEU:O	2.61	0.53
1:F:235:ILE:CG2	1:F:260:LEU:HG	2.38	0.53
1:A:67:SER:O	1:A:68:ASN:ND2	2.42	0.53
1:A:206:ARG:HD3	1:A:281:ASP:HB2	1.90	0.53
1:C:195:GLU:O	1:C:198:GLN:HB2	2.09	0.53
1:E:282:SER:OG	1:E:284:THR:OG1	2.26	0.53
1:F:253:PHE:O	1:F:254:ASP:CB	2.57	0.53
1:B:27:ASP:OD1	1:B:56:ARG:NH2	2.42	0.53
1:A:299:ILE:O	1:A:299:ILE:CG1	2.57	0.53
1:B:239:HIS:HB3	1:B:240:PRO:HD2	1.90	0.53
1:D:365:ASP:OD2	1:F:323:ASN:ND2	2.42	0.53
1:E:95:LEU:CD2	1:E:117:MET:HB3	2.39	0.53
1:F:146:PRO:HD2	1:F:166:PHE:O	2.08	0.53
1:C:50:PHE:CE1	1:C:58:PRO:HD3	2.44	0.53
1:D:249:SER:OG	1:D:250:LYS:N	2.39	0.53
1:E:59:ASP:O	1:E:60:HIS:CD2	2.62	0.53
1:E:298:LEU:HD22	1:E:300:ARG:HB2	1.90	0.53
1:D:13:ARG:HD3	1:D:49:PHE:CE2	2.44	0.53
1:F:137:VAL:HA	1:F:140:VAL:HG12	1.91	0.53
1:D:137:VAL:HA	1:D:140:VAL:HG12	1.91	0.53
1:E:133:ASN:O	1:E:137:VAL:HG12	2.09	0.53
1:E:246:ILE:C	1:E:246:ILE:HD12	2.34	0.53
1:F:247:GLU:OE2	1:F:247:GLU:HA	2.08	0.53
1:F:315:ILE:HD13	1:F:330:LEU:HD13	1.91	0.53
1:B:246:ILE:HB	1:B:253:PHE:HZ	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ASP:HB3	1:D:367:ILE:CD1	2.39	0.52
1:A:94:ILE:HG23	1:A:101:CYS:HB3	1.90	0.52
1:B:202:VAL:HG22	1:B:279:LEU:HB2	1.91	0.52
1:C:204:ALA:O	1:C:210:ILE:HD11	2.09	0.52
1:C:255:PRO:HD2	1:C:256:LEU:HD12	1.92	0.52
1:E:115:PHE:CE2	1:E:143:VAL:HG21	2.44	0.52
1:A:247:GLU:O	1:A:248:GLU:C	2.52	0.52
1:B:254:ASP:CB	1:B:255:PRO:HD2	2.40	0.52
1:D:212:ASN:C	1:D:212:ASN:HD22	2.18	0.52
1:D:4:LEU:N	1:F:326:GLN:NE2	2.57	0.52
1:C:95:LEU:HD22	1:C:117:MET:HB3	1.92	0.52
1:A:68:ASN:C	1:A:68:ASN:HD22	2.17	0.52
1:D:182:LYS:HD2	1:D:266:PHE:CE2	2.44	0.52
1:F:52:ASP:O	1:F:53:LEU:HB2	2.10	0.52
1:D:68:ASN:O	1:D:72:THR:HG22	2.10	0.52
1:D:305:ARG:NE	1:D:307:GLU:OE2	2.37	0.52
1:A:95:LEU:HD22	1:A:117:MET:CB	2.39	0.52
1:F:299:ILE:HG23	1:F:324:LEU:HD21	1.91	0.52
1:F:315:ILE:CD1	1:F:330:LEU:HD13	2.40	0.52
1:B:46:ASN:ND2	1:B:57:GLN:HE22	1.98	0.52
1:D:305:ARG:HD3	1:D:347:TYR:OH	2.10	0.52
1:A:68:ASN:ND2	1:A:68:ASN:C	2.68	0.51
1:D:121:ASN:O	1:D:122:ARG:HD3	2.09	0.51
1:F:62:LEU:O	1:F:63:GLU:C	2.52	0.51
1:B:64:ALA:O	1:B:65:VAL:CB	2.58	0.51
1:C:138:ASP:OD2	1:C:155:LEU:HD21	2.10	0.51
1:D:253:PHE:CZ	1:D:257:VAL:HG11	2.45	0.51
1:D:308:VAL:HG22	1:D:313:THR:CG2	2.41	0.51
1:E:142:ASP:HB3	1:E:367:ILE:HD13	1.92	0.51
1:D:207:GLU:O	1:D:208:GLU:CB	2.58	0.51
1:B:224:ASN:O	1:B:227:ALA:HB3	2.10	0.51
1:C:221:ASN:O	1:C:224:ASN:HB3	2.09	0.51
1:C:93:LEU:HD21	1:C:117:MET:HE2	1.92	0.51
1:D:224:ASN:HD21	1:D:253:PHE:CB	2.23	0.51
1:F:13:ARG:HB2	1:F:14:PRO:HD3	1.91	0.51
1:F:80:THR:HG21	1:F:103:ALA:CA	2.41	0.51
1:E:145:LEU:HD21	1:E:359:ILE:HG21	1.93	0.51
1:E:232:MET:HE1	1:E:276:PHE:HB2	1.92	0.51
1:F:300:ARG:O	1:F:318:GLY:HA2	2.11	0.51
1:B:212:ASN:HB3	1:B:215:ASN:ND2	2.25	0.51
1:E:236:TYR:CE1	1:E:238:THR:HB	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:313:THR:O	1:F:314:VAL:HB	2.10	0.51
1:A:358:LYS:HE3	1:E:334:MET:CE	2.35	0.51
1:F:268:TYR:O	1:F:271:LEU:HB3	2.10	0.51
1:A:339:GLU:CG	1:C:354:THR:HG21	2.41	0.50
1:A:358:LYS:HE2	1:E:334:MET:CE	2.41	0.50
1:F:311:LYS:HG3	1:F:344:ALA:HA	1.94	0.50
1:A:68:ASN:HD21	1:A:71:GLU:H	1.59	0.50
1:B:232:MET:O	1:B:256:LEU:HD12	2.11	0.50
1:D:330:LEU:O	1:D:334:MET:HB2	2.11	0.50
1:E:198:GLN:HA	1:E:198:GLN:HE21	1.76	0.50
1:C:76:ILE:O	1:C:80:THR:OG1	2.29	0.50
1:E:49:PHE:HB3	1:E:50:PHE:CD2	2.46	0.50
1:A:298:LEU:HD22	1:A:299:ILE:N	2.27	0.50
1:C:277:VAL:HG11	1:C:328:VAL:HG13	1.92	0.50
1:E:64:ALA:HA	1:E:79:LYS:HE3	1.92	0.50
1:F:59:ASP:C	1:F:60:HIS:CD2	2.90	0.50
1:A:74:GLY:HA2	1:B:74:GLY:HA2	1.94	0.50
1:B:237:SER:HB2	1:B:260:LEU:HD12	1.92	0.50
1:E:142:ASP:HB3	1:E:367:ILE:CD1	2.42	0.50
1:E:276:PHE:CZ	1:E:332:ARG:HB2	2.47	0.50
1:F:227:ALA:HB2	1:F:234:VAL:HG21	1.93	0.50
1:E:247:GLU:C	1:E:248:GLU:HG3	2.36	0.50
1:F:53:LEU:HD23	1:F:55:LEU:HD12	1.93	0.50
1:C:64:ALA:O	1:C:65:VAL:CG1	2.51	0.50
1:C:137:VAL:HA	1:C:140:VAL:HG12	1.92	0.50
1:E:17:ILE:O	1:E:20:SER:HB3	2.11	0.50
1:C:216:PHE:CZ	1:C:220:MET:HE2	2.46	0.50
1:D:123:CYS:HB2	1:D:302:SER:HB2	1.93	0.50
1:D:272:GLN:HB3	1:D:294:PHE:CE2	2.47	0.50
1:F:46:ASN:O	1:F:47:GLN:C	2.54	0.50
1:F:243:TRP:CZ2	1:F:259:GLN:HG2	2.47	0.50
1:D:225:ASP:OD2	1:D:321:TYR:OH	2.26	0.49
1:E:355:LYS:O	1:E:359:ILE:HG13	2.12	0.49
1:B:329:GLU:O	1:B:330:LEU:C	2.55	0.49
1:E:80:THR:HG21	1:E:103:ALA:HB1	1.92	0.49
1:E:281:ASP:HB3	1:E:299:ILE:HG13	1.92	0.49
1:F:51:ASP:O	1:F:54:GLU:N	2.45	0.49
1:F:190:ASN:O	1:F:191:LYS:C	2.54	0.49
1:B:345:ILE:HA	1:B:348:LYS:HE3	1.95	0.49
1:D:322:ASN:HD22	1:D:323:ASN:N	2.08	0.49
1:E:161:ASN:HD22	1:E:163:ALA:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:LEU:HD12	1:F:107:ALA:HB2	1.93	0.49
1:C:310:ASP:O	1:E:355:LYS:HD3	2.12	0.49
1:D:216:PHE:CZ	1:D:246:ILE:HG22	2.47	0.49
1:F:299:ILE:CG2	1:F:324:LEU:HD21	2.43	0.49
1:D:142:ASP:CB	1:D:367:ILE:HD12	2.43	0.49
1:D:147:TYR:CE1	1:D:171:PRO:HD3	2.47	0.49
1:C:311:LYS:HE2	1:C:345:ILE:HD12	1.94	0.49
1:D:179:HIS:C	1:D:181:ASP:N	2.68	0.49
1:E:14:PRO:O	1:E:18:ARG:HG3	2.13	0.49
1:E:13:ARG:HB2	1:E:14:PRO:HD3	1.94	0.49
1:C:183:ILE:HG22	1:C:184:ASN:HD22	1.76	0.49
1:A:255:PRO:HG2	1:A:256:LEU:HD12	1.95	0.49
1:B:180:ARG:O	1:B:181:ASP:C	2.56	0.49
1:B:252:GLU:O	1:B:253:PHE:C	2.55	0.49
1:C:236:TYR:O	1:C:260:LEU:HB2	2.12	0.49
1:D:40:ASN:O	1:D:41:TYR:C	2.55	0.49
1:D:80:THR:HG21	1:D:103:ALA:CB	2.42	0.49
1:E:215:ASN:ND2	1:E:319:ILE:HG21	2.28	0.49
1:F:147:TYR:O	1:F:169:GLY:HA2	2.13	0.49
1:A:95:LEU:CD2	1:A:117:MET:CB	2.91	0.49
1:B:210:ILE:HD11	1:B:238:THR:OG1	2.13	0.49
1:B:242:SER:O	1:B:246:ILE:N	2.45	0.49
1:B:332:ARG:CG	1:B:333:GLU:N	2.74	0.49
1:A:232:MET:O	1:A:256:LEU:HD23	2.12	0.48
1:E:161:ASN:HD22	1:E:161:ASN:C	2.21	0.48
1:E:16:ILE:O	1:E:20:SER:N	2.47	0.48
1:C:316:VAL:HB	1:E:362:SER:HB3	1.95	0.48
1:E:184:ASN:N	1:E:184:ASN:HD22	2.12	0.48
1:F:232:MET:HE1	1:F:276:PHE:HB3	1.95	0.48
1:F:254:ASP:OD1	1:F:255:PRO:CD	2.60	0.48
1:F:313:THR:O	1:F:313:THR:CG2	2.61	0.48
1:B:115:PHE:CE2	1:B:360:ILE:HA	2.48	0.48
1:C:123:CYS:HB2	1:C:302:SER:HB2	1.94	0.48
1:C:144:ASN:O	1:C:146:PRO:HD3	2.14	0.48
1:F:153:ARG:O	1:F:154:TYR:C	2.55	0.48
1:C:207:GLU:O	1:C:208:GLU:HB2	2.14	0.48
1:B:203:SER:O	1:B:280:SER:HA	2.14	0.48
1:B:242:SER:O	1:B:245:LYS:N	2.47	0.48
1:B:243:TRP:O	1:B:246:ILE:HG13	2.14	0.48
1:B:355:LYS:HE2	1:D:311:LYS:HA	1.95	0.48
1:C:68:ASN:O	1:C:72:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:LEU:HD21	1:D:117:MET:HE2	1.95	0.48
1:E:207:GLU:O	1:E:208:GLU:CB	2.61	0.48
1:E:280:SER:HB3	1:E:285:LEU:HG	1.96	0.48
1:D:161:ASN:C	1:D:161:ASN:HD22	2.22	0.48
1:D:161:ASN:HD22	1:D:163:ALA:H	1.61	0.48
1:F:251:PHE:O	1:F:252:GLU:C	2.57	0.48
1:B:131:GLU:HA	1:B:134:ARG:HD2	1.96	0.48
1:B:254:ASP:HB2	1:B:255:PRO:HD2	1.94	0.48
1:B:298:LEU:CD1	1:B:303:THR:HG23	2.44	0.48
1:B:334:MET:HE3	1:F:358:LYS:CE	2.43	0.48
1:D:207:GLU:O	1:D:208:GLU:HB2	2.14	0.48
1:F:43:TYR:C	1:F:45:LEU:H	2.22	0.48
1:A:133:ASN:O	1:A:135:LYS:N	2.47	0.48
1:C:65:VAL:HA	1:C:72:THR:OG1	2.14	0.48
1:E:207:GLU:C	1:E:208:GLU:CG	2.87	0.48
1:F:43:TYR:O	1:F:46:ASN:N	2.47	0.48
1:F:235:ILE:HD13	1:F:235:ILE:N	2.29	0.48
1:A:284:THR:O	1:A:288:GLU:HG2	2.13	0.47
1:B:214:LYS:O	1:B:216:PHE:N	2.47	0.47
1:C:253:PHE:O	1:C:253:PHE:CD2	2.67	0.47
1:E:27:ASP:OD1	1:E:56:ARG:NH2	2.47	0.47
1:E:307:GLU:OE2	1:E:347:TYR:OH	2.30	0.47
1:A:48:ILE:HA	1:A:52:ASP:HB2	1.96	0.47
1:F:190:ASN:O	1:F:192:LEU:N	2.48	0.47
1:D:224:ASN:ND2	1:D:253:PHE:CB	2.77	0.47
1:E:52:ASP:C	1:E:54:GLU:H	2.23	0.47
1:F:69:LEU:HA	1:F:72:THR:HG22	1.96	0.47
1:F:93:LEU:O	1:F:94:ILE:HG13	2.14	0.47
1:F:95:LEU:HD22	1:F:117:MET:CB	2.42	0.47
1:F:303:THR:HB	1:F:305:ARG:H	1.80	0.47
1:B:198:GLN:O	1:B:233:PRO:HD2	2.14	0.47
1:C:95:LEU:HD22	1:C:117:MET:CB	2.44	0.47
1:D:122:ARG:NH2	1:D:158:GLU:OE1	2.47	0.47
1:D:247:GLU:HA	1:D:251:PHE:CB	2.45	0.47
1:F:80:THR:HA	1:F:83:VAL:HG12	1.97	0.47
1:A:214:LYS:HD2	1:A:214:LYS:O	2.15	0.47
1:C:186:SER:OG	1:C:267:ASP:OD1	2.31	0.47
1:E:174:GLU:OE2	1:E:353:SER:OG	2.22	0.47
1:F:332:ARG:HG3	1:F:333:GLU:H	1.77	0.47
1:B:13:ARG:HB2	1:B:14:PRO:HD3	1.97	0.47
1:C:236:TYR:HD1	1:C:237:SER:N	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:GLU:O	1:E:208:GLU:CG	2.63	0.47
1:A:8:THR:CB	1:A:32:GLN:HE21	2.28	0.47
1:A:308:VAL:HG22	1:A:313:THR:HG21	1.97	0.47
1:C:40:ASN:O	1:C:42:ASP:N	2.47	0.47
1:C:62:LEU:O	1:C:63:GLU:C	2.57	0.47
1:A:319:ILE:O	1:A:320:THR:C	2.58	0.46
1:D:322:ASN:C	1:D:322:ASN:ND2	2.68	0.46
1:A:92:LEU:HD23	1:A:93:LEU:N	2.31	0.46
1:A:279:LEU:CD2	1:A:324:LEU:HD22	2.45	0.46
1:E:20:SER:OG	1:E:21:SER:N	2.47	0.46
1:B:4:LEU:C	1:B:4:LEU:HD23	2.41	0.46
1:B:14:PRO:O	1:B:18:ARG:HG3	2.14	0.46
1:C:305:ARG:N	1:C:306:PRO:CD	2.78	0.46
1:C:45:LEU:C	1:C:47:GLN:N	2.73	0.46
1:D:345:ILE:HG22	1:D:346:ASP:N	2.31	0.46
1:F:42:ASP:O	1:F:44:THR:N	2.48	0.46
1:A:4:LEU:HD21	1:A:360:ILE:HG22	1.97	0.46
1:C:69:LEU:O	1:D:81:TYR:CZ	2.69	0.46
1:C:46:ASN:H	1:C:46:ASN:HD22	1.64	0.46
1:B:14:PRO:O	1:B:18:ARG:CG	2.64	0.46
1:E:146:PRO:HD2	1:E:166:PHE:O	2.16	0.46
1:F:10:VAL:HG12	1:F:19:LEU:CD1	2.46	0.46
1:A:276:PHE:CE2	1:A:332:ARG:HG2	2.51	0.46
1:B:239:HIS:O	1:B:243:TRP:CD1	2.68	0.46
1:C:187:ASP:O	1:C:190:ASN:N	2.48	0.46
1:C:334:MET:HE3	1:E:358:LYS:HE3	1.96	0.46
1:D:47:GLN:OE1	1:D:57:GLN:NE2	2.48	0.46
1:C:352:VAL:O	1:C:356:VAL:HG23	2.15	0.46
1:E:308:VAL:HG22	1:E:313:THR:CG2	2.46	0.46
1:A:108:LYS:HD3	1:A:140:VAL:O	2.16	0.45
1:A:216:PHE:CZ	1:A:220:MET:HE2	2.52	0.45
1:C:9:ILE:HD12	1:C:92:LEU:HD21	1.97	0.45
1:E:187:ASP:O	1:E:189:LEU:N	2.49	0.45
1:E:308:VAL:HG22	1:E:313:THR:HG21	1.98	0.45
1:A:46:ASN:O	1:A:49:PHE:O	2.34	0.45
1:D:131:GLU:HA	1:D:134:ARG:HD2	1.98	0.45
1:D:235:ILE:HG23	1:D:260:LEU:HG	1.96	0.45
1:E:6:LEU:HD21	1:E:93:LEU:CB	2.44	0.45
1:A:361:GLN:HG3	1:E:330:LEU:CD1	2.46	0.45
1:B:4:LEU:N	1:D:326:GLN:NE2	2.64	0.45
1:F:232:MET:HE1	1:F:276:PHE:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:330:LEU:O	1:F:331:ALA:C	2.59	0.45
1:C:200:ILE:HG13	1:C:232:MET:HE2	1.97	0.45
1:D:243:TRP:O	1:D:246:ILE:HG13	2.17	0.45
1:F:299:ILE:O	1:F:300:ARG:HG3	2.16	0.45
1:A:133:ASN:O	1:A:134:ARG:C	2.59	0.45
1:B:80:THR:HG21	1:B:103:ALA:CB	2.46	0.45
1:D:273:LYS:HA	1:D:294:PHE:HD2	1.82	0.45
1:D:372:TRP:O	1:D:373:ARG:O	2.33	0.45
1:E:66:GLY:O	1:E:67:SER:C	2.59	0.45
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.83	0.45
1:B:28:GLN:HB2	1:B:29:TYR:CD2	2.52	0.45
1:D:66:GLY:O	1:D:67:SER:C	2.60	0.45
1:E:284:THR:O	1:E:285:LEU:C	2.60	0.45
1:F:248:GLU:O	1:F:251:PHE:HD2	2.00	0.45
1:E:9:ILE:HG13	1:E:92:LEU:HD21	1.98	0.45
1:F:287:GLU:O	1:F:291:ILE:HG13	2.16	0.45
1:A:253:PHE:O	1:A:254:ASP:C	2.59	0.45
1:C:81:TYR:CE2	1:C:110:LEU:HD21	2.52	0.45
1:D:284:THR:O	1:D:285:LEU:C	2.60	0.45
1:E:95:LEU:HD13	1:E:96:GLY:N	2.32	0.45
1:F:144:ASN:ND2	1:F:160:PHE:CZ	2.85	0.45
1:A:215:ASN:ND2	1:A:319:ILE:CD1	2.72	0.45
1:C:92:LEU:HD12	1:C:107:ALA:CB	2.47	0.45
1:D:177:GLU:C	1:D:179:HIS:H	2.25	0.45
1:E:188:VAL:O	1:E:192:LEU:HG	2.16	0.45
1:E:298:LEU:CD1	1:E:303:THR:HG23	2.47	0.45
1:E:319:ILE:O	1:E:319:ILE:CG2	2.65	0.45
1:F:228:LYS:O	1:F:231:LYS:HE3	2.16	0.45
1:C:201:LEU:HD12	1:C:201:LEU:C	2.42	0.44
1:D:55:LEU:HD23	1:D:55:LEU:HA	1.85	0.44
1:D:252:GLU:O	1:D:253:PHE:C	2.60	0.44
1:F:173:THR:HG22	1:F:291:ILE:HG12	1.99	0.44
1:C:13:ARG:HB2	1:C:14:PRO:HD3	1.99	0.44
1:C:66:GLY:H	1:C:72:THR:HB	1.81	0.44
1:D:92:LEU:C	1:D:92:LEU:CD2	2.91	0.44
1:D:232:MET:HE1	1:D:276:PHE:HB2	1.99	0.44
1:A:306:PRO:C	1:A:308:VAL:H	2.25	0.44
1:B:214:LYS:O	1:B:215:ASN:C	2.61	0.44
1:B:334:MET:HE3	1:F:358:LYS:HE3	1.99	0.44
1:B:340:PRO:HG2	1:F:351:ASN:HB3	1.99	0.44
1:D:224:ASN:CG	1:D:253:PHE:HB2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:LEU:HD12	1:E:107:ALA:HB2	1.99	0.44
1:C:235:ILE:HG22	1:C:260:LEU:CG	2.40	0.44
1:F:195:GLU:HB2	1:F:198:GLN:HG3	1.99	0.44
1:C:209:ASN:ND2	1:C:319:ILE:HD11	2.33	0.44
1:D:85:LEU:O	1:D:88:GLN:HG2	2.18	0.44
1:D:284:THR:HB	1:D:288:GLU:CD	2.43	0.44
1:E:187:ASP:OD1	1:E:188:VAL:N	2.50	0.44
1:F:225:ASP:OD1	1:F:225:ASP:N	2.50	0.44
1:F:330:LEU:HD22	1:F:334:MET:HE2	1.99	0.44
1:C:253:PHE:O	1:C:253:PHE:HD2	2.01	0.44
1:D:42:ASP:O	1:D:46:ASN:HB2	2.18	0.44
1:F:64:ALA:O	1:F:65:VAL:HB	2.16	0.44
1:A:306:PRO:C	1:A:308:VAL:N	2.75	0.44
1:B:93:LEU:HD21	1:B:117:MET:HE2	1.99	0.44
1:B:280:SER:OG	1:B:282:SER:HB3	2.17	0.44
1:C:260:LEU:HD23	1:C:260:LEU:HA	1.80	0.44
1:D:242:SER:O	1:D:243:TRP:C	2.60	0.44
1:D:250:LYS:HA	1:D:252:GLU:OE1	2.18	0.44
1:A:307:GLU:OE1	1:A:307:GLU:N	2.46	0.44
1:D:265:PHE:CE1	1:D:269:ASN:ND2	2.86	0.44
1:E:40:ASN:O	1:E:43:TYR:HB3	2.17	0.44
1:E:177:GLU:C	1:E:179:HIS:H	2.25	0.44
1:D:80:THR:HG21	1:D:103:ALA:HB1	1.99	0.44
1:D:94:ILE:HD11	1:D:103:ALA:HB3	2.00	0.44
1:F:224:ASN:O	1:F:227:ALA:N	2.51	0.44
1:F:330:LEU:HD22	1:F:334:MET:CE	2.48	0.44
1:B:254:ASP:OD2	1:B:254:ASP:C	2.61	0.43
1:F:161:ASN:C	1:F:161:ASN:HD22	2.25	0.43
1:F:236:TYR:CE1	1:F:238:THR:HB	2.53	0.43
1:A:43:TYR:CD1	1:A:43:TYR:C	2.96	0.43
1:A:121:ASN:O	1:A:134:ARG:HD3	2.18	0.43
1:B:137:VAL:HA	1:B:140:VAL:HG12	2.01	0.43
1:A:4:LEU:CD1	1:A:90:ASP:HB2	2.48	0.43
1:A:224:ASN:O	1:A:227:ALA:HB3	2.19	0.43
1:A:284:THR:O	1:A:288:GLU:HG3	2.18	0.43
1:A:294:PHE:C	1:A:294:PHE:CD2	2.96	0.43
1:C:8:THR:HG1	1:C:32:GLN:HE21	1.62	0.43
1:E:13:ARG:HD3	1:E:50:PHE:CZ	2.52	0.43
1:E:292:LEU:O	1:E:293:LYS:C	2.61	0.43
1:F:13:ARG:HD3	1:F:50:PHE:CE2	2.52	0.43
1:F:322:ASN:C	1:F:322:ASN:HD22	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD13	1:A:196:PRO:HD3	2.00	0.43
1:A:246:ILE:HD12	1:A:246:ILE:O	2.17	0.43
1:B:45:LEU:HD22	1:B:45:LEU:HA	1.89	0.43
1:C:313:THR:O	1:C:313:THR:CG2	2.65	0.43
1:C:334:MET:HE3	1:E:358:LYS:CE	2.48	0.43
1:D:209:ASN:ND2	1:D:299:ILE:O	2.51	0.43
1:D:352:VAL:O	1:D:356:VAL:HG23	2.18	0.43
1:A:45:LEU:HD22	1:A:45:LEU:O	2.19	0.43
1:B:121:ASN:O	1:B:134:ARG:HD3	2.18	0.43
1:D:202:VAL:HG22	1:D:279:LEU:HD13	2.01	0.43
1:D:247:GLU:HG2	1:D:251:PHE:CB	2.48	0.43
1:E:198:GLN:HA	1:E:198:GLN:NE2	2.32	0.43
1:F:24:LYS:O	1:F:28:GLN:HG3	2.18	0.43
1:F:45:LEU:HD23	1:F:45:LEU:HA	1.88	0.43
1:B:144:ASN:ND2	1:B:160:PHE:CE2	2.87	0.43
1:B:230:TYR:HE1	1:B:332:ARG:HD3	1.83	0.43
1:B:319:ILE:HD13	1:B:319:ILE:HA	1.90	0.43
1:C:46:ASN:HD22	1:C:46:ASN:N	2.16	0.43
1:D:176:ILE:O	1:D:180:ARG:N	2.50	0.43
1:F:48:ILE:HG13	1:F:49:PHE:H	1.83	0.43
1:A:13:ARG:CB	1:A:14:PRO:HD3	2.48	0.43
1:A:48:ILE:O	1:A:53:LEU:HB2	2.18	0.43
1:A:73:MET:SD	1:B:109:ARG:HD2	2.59	0.43
1:B:334:MET:HG3	1:B:339:GLU:HG3	1.99	0.43
1:C:37:THR:HA	1:C:62:LEU:HB2	2.00	0.43
1:C:183:ILE:HG22	1:C:184:ASN:ND2	2.34	0.43
1:E:200:ILE:HG13	1:E:232:MET:HE2	1.99	0.43
1:F:294:PHE:CD1	1:F:294:PHE:C	2.96	0.43
1:F:315:ILE:CD1	1:F:330:LEU:HB3	2.49	0.43
1:B:200:ILE:O	1:B:234:VAL:HA	2.18	0.43
1:C:40:ASN:C	1:C:42:ASP:H	2.27	0.43
1:D:286:SER:O	1:D:308:VAL:HG21	2.18	0.43
1:E:264:GLY:O	1:E:266:PHE:N	2.52	0.43
1:A:285:LEU:O	1:A:286:SER:C	2.61	0.43
1:C:26:CYS:O	1:C:30:PHE:HB2	2.18	0.43
1:D:25:ALA:O	1:D:29:TYR:HD2	2.01	0.43
1:D:372:TRP:O	1:D:373:ARG:C	2.61	0.43
1:E:64:ALA:O	1:E:65:VAL:CB	2.65	0.43
1:E:290:SER:HB2	1:E:313:THR:HG21	2.01	0.43
1:B:358:LYS:HE3	1:D:334:MET:HE3	1.97	0.43
1:C:92:LEU:HD12	1:C:107:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:THR:O	1:A:76:ILE:HG13	2.19	0.42
1:A:332:ARG:HA	1:A:332:ARG:HD2	1.37	0.42
1:B:253:PHE:O	1:B:254:ASP:CB	2.67	0.42
1:B:303:THR:HB	1:B:305:ARG:H	1.84	0.42
1:C:33:ILE:O	1:C:33:ILE:HG22	2.18	0.42
1:C:69:LEU:HA	1:C:72:THR:CG2	2.49	0.42
1:D:199:TYR:CA	1:D:232:MET:HE3	2.49	0.42
1:B:161:ASN:ND2	1:B:163:ALA:H	2.17	0.42
1:F:1:MET:O	1:F:2:GLU:OE1	2.37	0.42
1:F:334:MET:CG	1:F:339:GLU:HG3	2.45	0.42
1:A:339:GLU:HG2	1:C:354:THR:HG21	2.01	0.42
1:B:237:SER:HB3	1:B:260:LEU:HD12	2.00	0.42
1:D:81:TYR:CE2	1:D:110:LEU:HD21	2.54	0.42
1:D:247:GLU:HA	1:D:251:PHE:HB2	2.01	0.42
1:E:6:LEU:CD2	1:E:6:LEU:C	2.92	0.42
1:E:276:PHE:CD1	1:E:335:GLN:NE2	2.87	0.42
1:E:319:ILE:O	1:E:319:ILE:HG22	2.20	0.42
1:F:13:ARG:HD3	1:F:50:PHE:CZ	2.55	0.42
1:F:43:TYR:C	1:F:45:LEU:N	2.77	0.42
1:A:164:ASN:HD22	1:A:164:ASN:N	2.18	0.42
1:B:294:PHE:CD1	1:B:294:PHE:C	2.98	0.42
1:C:45:LEU:H	1:C:45:LEU:HG	1.47	0.42
1:D:93:LEU:HD22	1:D:94:ILE:N	2.33	0.42
1:D:40:ASN:O	1:D:42:ASP:N	2.52	0.42
1:D:219:LEU:O	1:D:222:ALA:HB3	2.20	0.42
1:C:203:SER:HA	1:C:237:SER:O	2.19	0.42
1:E:80:THR:HA	1:E:83:VAL:HG12	2.02	0.42
1:E:216:PHE:CZ	1:E:220:MET:HE2	2.55	0.42
1:D:179:HIS:O	1:D:180:ARG:C	2.63	0.42
1:F:48:ILE:HD12	1:F:49:PHE:CD2	2.54	0.42
1:F:49:PHE:O	1:F:52:ASP:O	2.38	0.42
1:F:94:ILE:HG22	1:F:116:HIS:HA	2.02	0.42
1:F:220:MET:HE1	1:F:236:TYR:OH	2.20	0.42
1:F:250:LYS:HE3	1:F:250:LYS:HB3	1.88	0.42
1:B:13:ARG:N	1:B:14:PRO:CD	2.82	0.42
1:B:329:GLU:OE2	1:B:332:ARG:NH1	2.52	0.42
1:B:339:GLU:OE2	1:F:29:TYR:OH	2.28	0.42
1:D:1:MET:SD	1:D:1:MET:N	2.89	0.42
1:D:220:MET:HE1	1:D:236:TYR:CZ	2.55	0.42
1:C:73:MET:HE1	1:D:109:ARG:HH11	1.85	0.42
1:D:230:TYR:HE1	1:D:332:ARG:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:PHE:CE2	1:E:360:ILE:HA	2.55	0.42
1:F:366:ILE:HG23	1:F:370:ASN:ND2	2.35	0.42
1:B:144:ASN:ND2	1:B:160:PHE:CZ	2.88	0.41
1:B:239:HIS:CB	1:B:240:PRO:HD2	2.49	0.41
1:B:369:ARG:O	1:B:373:ARG:HA	2.20	0.41
1:C:329:GLU:O	1:C:333:GLU:HB2	2.20	0.41
1:D:319:ILE:HD13	1:D:319:ILE:HA	1.88	0.41
1:E:211:ASP:O	1:E:213:GLU:N	2.53	0.41
1:E:280:SER:CB	1:E:285:LEU:HG	2.50	0.41
1:F:62:LEU:O	1:F:64:ALA:N	2.52	0.41
1:A:49:PHE:CZ	1:A:58:PRO:HD3	2.55	0.41
1:F:45:LEU:O	1:F:48:ILE:CG1	2.64	0.41
1:A:253:PHE:CD1	1:A:257:VAL:HG11	2.55	0.41
1:B:65:VAL:CA	1:B:72:THR:HB	2.46	0.41
1:C:225:ASP:O	1:C:229:LYS:HB2	2.20	0.41
1:C:131:GLU:HA	1:C:134:ARG:HD2	2.02	0.41
1:D:123:CYS:O	1:D:124:PHE:HB2	2.20	0.41
1:F:119:ALA:HB1	1:F:144:ASN:HB3	2.02	0.41
1:F:187:ASP:O	1:F:190:ASN:N	2.54	0.41
1:F:235:ILE:HG22	1:F:260:LEU:HG	2.02	0.41
1:D:95:LEU:HD13	1:D:95:LEU:C	2.46	0.41
1:D:369:ARG:NH1	1:F:301:THR:HB	2.35	0.41
1:A:78:ALA:O	1:A:81:TYR:HB3	2.20	0.41
1:D:49:PHE:CD1	1:D:49:PHE:C	2.99	0.41
1:E:19:LEU:HD11	1:E:95:LEU:HB2	2.03	0.41
1:A:26:CYS:O	1:A:30:PHE:HB2	2.20	0.41
1:A:109:ARG:HD2	1:B:73:MET:HE1	2.02	0.41
1:B:106:SER:O	1:B:107:ALA:C	2.63	0.41
1:B:334:MET:SD	1:F:354:THR:HG22	2.60	0.41
1:C:335:GLN:OE1	1:C:335:GLN:HA	2.21	0.41
1:D:64:ALA:O	1:D:65:VAL:CB	2.67	0.41
1:D:168:THR:O	1:D:352:VAL:HG22	2.20	0.41
1:E:284:THR:HB	1:E:288:GLU:CD	2.46	0.41
1:F:50:PHE:CD2	1:F:50:PHE:N	2.87	0.41
1:A:347:TYR:N	1:A:347:TYR:CD1	2.89	0.41
1:B:187:ASP:O	1:B:188:VAL:C	2.63	0.41
1:D:246:ILE:HD12	1:D:246:ILE:C	2.45	0.41
1:F:149:GLU:O	1:F:150:HIS:C	2.63	0.41
1:A:252:GLU:O	1:A:253:PHE:C	2.64	0.41
1:B:7:MET:O	1:B:92:LEU:HA	2.21	0.41
1:B:185:HIS:O	1:B:186:SER:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LEU:HD23	1:B:260:LEU:HA	1.87	0.41
1:B:325:ILE:HG22	1:B:326:GLN:N	2.35	0.41
1:C:81:TYR:CE1	1:C:85:LEU:HD12	2.56	0.41
1:E:24:LYS:HE2	1:E:54:GLU:O	2.21	0.41
1:E:74:GLY:HA3	1:F:74:GLY:O	2.21	0.41
1:E:243:TRP:HA	1:E:246:ILE:HG13	2.02	0.41
1:B:342:ILE:HD12	1:F:351:ASN:OD1	2.21	0.41
1:C:87:GLU:O	1:C:88:GLN:C	2.64	0.41
1:A:143:VAL:O	1:A:143:VAL:HG12	2.21	0.40
1:B:64:ALA:O	1:B:65:VAL:HG12	2.21	0.40
1:B:92:LEU:HD12	1:B:107:ALA:HB2	2.03	0.40
1:C:144:ASN:ND2	1:C:160:PHE:CZ	2.89	0.40
1:C:198:GLN:C	1:C:232:MET:HE3	2.46	0.40
1:D:13:ARG:N	1:D:14:PRO:CD	2.84	0.40
1:D:123:CYS:HB3	1:D:304:GLU:OE1	2.21	0.40
1:D:170:SER:OG	1:D:287:GLU:OE2	2.32	0.40
1:D:236:TYR:CD1	1:D:236:TYR:C	2.97	0.40
1:E:40:ASN:HB2	1:E:61:TYR:CD2	2.55	0.40
1:F:43:TYR:O	1:F:45:LEU:N	2.54	0.40
1:F:212:ASN:C	1:F:212:ASN:ND2	2.69	0.40
1:A:68:ASN:ND2	1:A:71:GLU:HB2	2.36	0.40
1:B:225:ASP:OD1	1:B:225:ASP:N	2.53	0.40
1:C:81:TYR:CZ	1:C:110:LEU:HD21	2.56	0.40
1:F:265:PHE:CE1	1:F:269:ASN:ND2	2.87	0.40
1:A:170:SER:HA	1:A:171:PRO:HD3	1.96	0.40
1:B:188:VAL:HG13	1:B:189:LEU:N	2.36	0.40
1:B:251:PHE:CD1	1:B:251:PHE:O	2.74	0.40
1:C:187:ASP:C	1:C:189:LEU:N	2.77	0.40
1:D:110:LEU:O	1:D:111:LYS:C	2.64	0.40
1:D:207:GLU:O	1:D:208:GLU:HG3	2.20	0.40
1:F:183:ILE:HG22	1:F:184:ASN:ND2	2.37	0.40
1:C:118:GLU:HG3	1:C:147:TYR:CE2	2.56	0.40
1:C:207:GLU:O	1:C:208:GLU:CB	2.69	0.40
1:C:224:ASN:OD1	1:C:253:PHE:HA	2.20	0.40
1:D:253:PHE:CE1	1:D:257:VAL:HG11	2.57	0.40
1:D:363:TYR:HA	1:D:366:ILE:HB	2.02	0.40
1:E:40:ASN:OD1	1:E:43:TYR:HB3	2.21	0.40
1:F:76:ILE:O	1:F:80:THR:HB	2.22	0.40
1:F:116:HIS:CE1	1:F:119:ALA:HA	2.56	0.40
1:F:176:ILE:CG2	1:F:292:LEU:HD21	2.52	0.40
1:F:202:VAL:HA	1:F:279:LEU:O	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	368/374 (98%)	301 (82%)	55 (15%)	12 (3%)	3	21
1	B	372/374 (100%)	305 (82%)	50 (13%)	17 (5%)	2	15
1	C	372/374 (100%)	311 (84%)	45 (12%)	16 (4%)	2	16
1	D	372/374 (100%)	312 (84%)	46 (12%)	14 (4%)	2	18
1	E	372/374 (100%)	306 (82%)	52 (14%)	14 (4%)	2	18
1	F	372/374 (100%)	299 (80%)	55 (15%)	18 (5%)	2	14
All	All	2228/2244 (99%)	1834 (82%)	303 (14%)	91 (4%)	2	17

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	134	ARG
1	A	140	VAL
1	A	252	GLU
1	A	254	ASP
1	B	65	VAL
1	B	215	ASN
1	B	253	PHE
1	B	254	ASP
1	B	293	LYS
1	C	43	TYR
1	C	162	LYS
1	C	188	VAL
1	C	248	GLU
1	C	252	GLU
1	D	41	TYR
1	D	42	ASP

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Mol	Chain	Res	Type
1	D	65	VAL
1	D	67	SER
1	D	69	LEU
1	D	373	ARG
1	E	65	VAL
1	E	69	LEU
1	E	212	ASN
1	E	265	PHE
1	E	285	LEU
1	E	293	LYS
1	F	2	GLU
1	F	47	GLN
1	F	53	LEU
1	F	191	LYS
1	F	254	ASP
1	F	314	VAL
1	A	136	ILE
1	A	247	GLU
1	A	248	GLU
1	B	64	ALA
1	B	69	LEU
1	B	107	ALA
1	B	188	VAL
1	C	11	GLY
1	C	41	TYR
1	C	53	LEU
1	C	65	VAL
1	C	264	GLY
1	D	180	ARG
1	D	208	GLU
1	D	253	PHE
1	E	67	SER
1	E	188	VAL
1	F	11	GLY
1	F	43	TYR
1	F	44	THR
1	F	65	VAL
1	F	252	GLU
1	A	251	PHE
1	B	249	SER
1	B	264	GLY
1	C	2	GLU

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Mol	Chain	Res	Type
1	C	46	ASN
1	C	253	PHE
1	D	11	GLY
1	D	249	SER
1	E	231	LYS
1	F	20	SER
1	F	94	ILE
1	A	11	GLY
1	A	37	THR
1	A	307	GLU
1	B	11	GLY
1	B	214	LYS
1	D	2	GLU
1	D	212	ASN
1	D	254	ASP
1	E	284	THR
1	E	373	ARG
1	F	63	GLU
1	B	330	LEU
1	C	182	LYS
1	E	11	GLY
1	E	254	ASP
1	F	86	ARG
1	F	224	ASN
1	B	325	ILE
1	C	254	ASP
1	F	48	ILE
1	B	136	ILE
1	B	299	ILE
1	E	235	ILE
1	F	74	GLY
1	C	235	ILE

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	339/341 (99%)	280 (83%)	59 (17%)	2	10
1	B	341/341 (100%)	283 (83%)	58 (17%)	2	11
1	C	341/341 (100%)	285 (84%)	56 (16%)	2	12
1	D	341/341 (100%)	277 (81%)	64 (19%)	1	9
1	E	341/341 (100%)	281 (82%)	60 (18%)	2	10
1	F	341/341 (100%)	279 (82%)	62 (18%)	2	9
All	All	2044/2046 (100%)	1685 (82%)	359 (18%)	2	10

All (359) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	13	ARG
1	A	16	ILE
1	A	43	TYR
1	A	45	LEU
1	A	48	ILE
1	A	51	ASP
1	A	53	LEU
1	A	55	LEU
1	A	65	VAL
1	A	68	ASN
1	A	69	LEU
1	A	76	ILE
1	A	77	ILE
1	A	80	THR
1	A	92	LEU
1	A	93	LEU
1	A	94	ILE
1	A	95	LEU
1	A	101	CYS
1	A	109	ARG
1	A	137	VAL
1	A	140	VAL
1	A	143	VAL
1	A	162	LYS
1	A	201	LEU
1	A	208	GLU
1	A	214	LYS
1	A	215	ASN
1	A	219	LEU

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Mol	Chain	Res	Type
1	A	220	MET
1	A	223	ILE
1	A	237	SER
1	A	242	SER
1	A	246	ILE
1	A	247	GLU
1	A	248	GLU
1	A	252	GLU
1	A	260	LEU
1	A	261	LYS
1	A	271	LEU
1	A	285	LEU
1	A	288	GLU
1	A	298	LEU
1	A	299	ILE
1	A	303	THR
1	A	308	VAL
1	A	311	LYS
1	A	313	THR
1	A	314	VAL
1	A	325	ILE
1	A	329	GLU
1	A	332	ARG
1	A	333	GLU
1	A	343	ASP
1	A	348	LYS
1	A	354	THR
1	A	357	VAL
1	A	359	ILE
1	B	1	MET
1	B	6	LEU
1	B	18	ARG
1	B	33	ILE
1	B	39	GLN
1	B	45	LEU
1	B	51	ASP
1	B	55	LEU
1	B	56	ARG
1	B	65	VAL
1	B	69	LEU
1	B	72	THR
1	B	80	THR

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Mol	Chain	Res	Type
1	B	85	LEU
1	B	92	LEU
1	B	93	LEU
1	B	95	LEU
1	B	109	ARG
1	B	161	ASN
1	B	180	ARG
1	B	192	LEU
1	B	198	GLN
1	B	209	ASN
1	B	210	ILE
1	B	213	GLU
1	B	218	SER
1	B	220	MET
1	B	225	ASP
1	B	229	LYS
1	B	232	MET
1	B	237	SER
1	B	242	SER
1	B	245	LYS
1	B	250	LYS
1	B	254	ASP
1	B	256	LEU
1	B	263	PHE
1	B	285	LEU
1	B	286	SER
1	B	290	SER
1	B	297	VAL
1	B	298	LEU
1	B	299	ILE
1	B	301	THR
1	B	303	THR
1	B	308	VAL
1	B	309	LEU
1	B	313	THR
1	B	314	VAL
1	B	324	LEU
1	B	325	ILE
1	B	330	LEU
1	B	332	ARG
1	B	342	ILE
1	B	345	ILE

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Mol	Chain	Res	Type
1	B	359	ILE
1	B	364	LYS
1	B	365	ASP
1	C	1	MET
1	C	6	LEU
1	C	16	ILE
1	C	37	THR
1	C	39	GLN
1	C	44	THR
1	C	45	LEU
1	C	46	ASN
1	C	47	GLN
1	C	48	ILE
1	C	53	LEU
1	C	56	ARG
1	C	85	LEU
1	C	92	LEU
1	C	93	LEU
1	C	95	LEU
1	C	97	ASP
1	C	101	CYS
1	C	109	ARG
1	C	138	ASP
1	C	165	ILE
1	C	173	THR
1	C	177	GLU
1	C	180	ARG
1	C	191	LYS
1	C	195	GLU
1	C	201	LEU
1	C	207	GLU
1	C	210	ILE
1	C	217	LYS
1	C	220	MET
1	C	221	ASN
1	C	232	MET
1	C	242	SER
1	C	249	SER
1	C	251	PHE
1	C	253	PHE
1	C	254	ASP
1	C	260	LEU

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Mol	Chain	Res	Type
1	C	261	LYS
1	C	266	PHE
1	C	284	THR
1	C	285	LEU
1	C	298	LEU
1	C	299	ILE
1	C	303	THR
1	C	308	VAL
1	C	313	THR
1	C	314	VAL
1	C	319	ILE
1	C	324	LEU
1	C	325	ILE
1	C	330	LEU
1	C	336	ASN
1	C	342	ILE
1	C	369	ARG
1	D	1	MET
1	D	21	SER
1	D	33	ILE
1	D	39	GLN
1	D	40	ASN
1	D	42	ASP
1	D	46	ASN
1	D	48	ILE
1	D	52	ASP
1	D	53	LEU
1	D	56	ARG
1	D	69	LEU
1	D	72	THR
1	D	77	ILE
1	D	92	LEU
1	D	93	LEU
1	D	94	ILE
1	D	97	ASP
1	D	101	CYS
1	D	109	ARG
1	D	127	ASN
1	D	161	ASN
1	D	165	ILE
1	D	180	ARG
1	D	205	HIS

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Mol	Chain	Res	Type
1	D	210	ILE
1	D	212	ASN
1	D	218	SER
1	D	220	MET
1	D	229	LYS
1	D	231	LYS
1	D	237	SER
1	D	246	ILE
1	D	250	LYS
1	D	251	PHE
1	D	252	GLU
1	D	253	PHE
1	D	254	ASP
1	D	258	LYS
1	D	261	LYS
1	D	273	LYS
1	D	280	SER
1	D	284	THR
1	D	285	LEU
1	D	286	SER
1	D	298	LEU
1	D	302	SER
1	D	303	THR
1	D	308	VAL
1	D	309	LEU
1	D	313	THR
1	D	314	VAL
1	D	319	ILE
1	D	322	ASN
1	D	324	LEU
1	D	330	LEU
1	D	332	ARG
1	D	334	MET
1	D	335	GLN
1	D	342	ILE
1	D	345	ILE
1	D	357	VAL
1	D	364	LYS
1	D	367	ILE
1	E	1	MET
1	E	2	GLU
1	E	6	LEU

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Mol	Chain	Res	Type
1	E	33	ILE
1	E	47	GLN
1	E	48	ILE
1	E	55	LEU
1	E	56	ARG
1	E	59	ASP
1	E	65	VAL
1	E	69	LEU
1	E	92	LEU
1	E	93	LEU
1	E	94	ILE
1	E	100	SER
1	E	109	ARG
1	E	135	LYS
1	E	142	ASP
1	E	145	LEU
1	E	161	ASN
1	E	176	ILE
1	E	180	ARG
1	E	181	ASP
1	E	188	VAL
1	E	191	LYS
1	E	201	LEU
1	E	203	SER
1	E	207	GLU
1	E	208	GLU
1	E	214	LYS
1	E	217	LYS
1	E	218	SER
1	E	220	MET
1	E	232	MET
1	E	239	HIS
1	E	242	SER
1	E	247	GLU
1	E	250	LYS
1	E	253	PHE
1	E	260	LEU
1	E	261	LYS
1	E	280	SER
1	E	285	LEU
1	E	298	LEU
1	E	303	THR

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Mol	Chain	Res	Type
1	E	304	GLU
1	E	308	VAL
1	E	313	THR
1	E	314	VAL
1	E	324	LEU
1	E	330	LEU
1	E	334	MET
1	E	335	GLN
1	E	342	ILE
1	E	345	ILE
1	E	359	ILE
1	E	364	LYS
1	E	366	ILE
1	E	367	ILE
1	E	369	ARG
1	F	1	MET
1	F	6	LEU
1	F	37	THR
1	F	39	GLN
1	F	47	GLN
1	F	48	ILE
1	F	55	LEU
1	F	57	GLN
1	F	69	LEU
1	F	77	ILE
1	F	85	LEU
1	F	92	LEU
1	F	93	LEU
1	F	94	ILE
1	F	95	LEU
1	F	97	ASP
1	F	100	SER
1	F	117	MET
1	F	145	LEU
1	F	157	ASP
1	F	177	GLU
1	F	191	LYS
1	F	198	GLN
1	F	212	ASN
1	F	217	LYS
1	F	220	MET
1	F	224	ASN

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Mol	Chain	Res	Type
1	F	225	ASP
1	F	232	MET
1	F	235	ILE
1	F	239	HIS
1	F	241	ARG
1	F	242	SER
1	F	244	LYS
1	F	245	LYS
1	F	246	ILE
1	F	249	SER
1	F	250	LYS
1	F	252	GLU
1	F	253	PHE
1	F	257	VAL
1	F	260	LEU
1	F	261	LYS
1	F	266	PHE
1	F	285	LEU
1	F	292	LEU
1	F	298	LEU
1	F	299	ILE
1	F	303	THR
1	F	308	VAL
1	F	314	VAL
1	F	319	ILE
1	F	324	LEU
1	F	327	SER
1	F	330	LEU
1	F	334	MET
1	F	335	GLN
1	F	342	ILE
1	F	345	ILE
1	F	354	THR
1	F	357	VAL
1	F	369	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	31	ASN
1	A	68	ASN

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Mol	Chain	Res	Type
1	A	75	ASN
1	A	164	ASN
1	A	198	GLN
1	A	209	ASN
1	A	215	ASN
1	A	361	GLN
1	B	46	ASN
1	B	75	ASN
1	B	144	ASN
1	B	161	ASN
1	B	164	ASN
1	B	184	ASN
1	B	190	ASN
1	B	212	ASN
1	B	272	GLN
1	B	326	GLN
1	B	336	ASN
1	B	370	ASN
1	C	32	GLN
1	C	39	GLN
1	C	46	ASN
1	C	75	ASN
1	C	99	ASN
1	C	161	ASN
1	C	179	HIS
1	C	184	ASN
1	C	198	GLN
1	C	209	ASN
1	C	239	HIS
1	C	322	ASN
1	C	323	ASN
1	C	326	GLN
1	D	28	GLN
1	D	32	GLN
1	D	40	ASN
1	D	75	ASN
1	D	144	ASN
1	D	161	ASN
1	D	164	ASN
1	D	184	ASN
1	D	212	ASN
1	D	224	ASN

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Mol	Chain	Res	Type
1	D	269	ASN
1	D	272	GLN
1	D	322	ASN
1	D	336	ASN
1	E	28	GLN
1	E	32	GLN
1	E	47	GLN
1	E	75	ASN
1	E	144	ASN
1	E	161	ASN
1	E	164	ASN
1	E	184	ASN
1	E	198	GLN
1	E	205	HIS
1	E	239	HIS
1	E	272	GLN
1	E	326	GLN
1	E	335	GLN
1	E	336	ASN
1	F	28	GLN
1	F	39	GLN
1	F	75	ASN
1	F	161	ASN
1	F	164	ASN
1	F	184	ASN
1	F	198	GLN
1	F	212	ASN
1	F	224	ASN
1	F	322	ASN
1	F	323	ASN
1	F	326	GLN
1	F	361	GLN
1	F	368	ASN
1	F	370	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
1	A	372/374 (99%)	-0.63	0	100	100	32, 60, 105, 136	0
1	B	374/374 (100%)	-0.56	0	100	100	34, 65, 122, 161	0
1	C	374/374 (100%)	-0.50	0	100	100	35, 69, 115, 144	0
1	D	374/374 (100%)	-0.56	1 (0%)	90	81	35, 66, 124, 189	0
1	E	374/374 (100%)	-0.52	1 (0%)	90	81	42, 69, 129, 179	0
1	F	374/374 (100%)	-0.46	0	100	100	41, 74, 125, 185	0
All	All	2242/2244 (99%)	-0.54	2 (0%)	92	89	32, 67, 121, 189	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	251	PHE	2.4
1	E	48	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.