Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 07:26 AM EDT

PDB ID	:	1PZN
Title	:	Rad51 (RadA)
Authors	:	Shin, D.S.; Tainer, J.A.
Deposited on	:	2003-07-12
Resolution	:	2.85 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 (i) 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 (i)) were used in the production of this report:

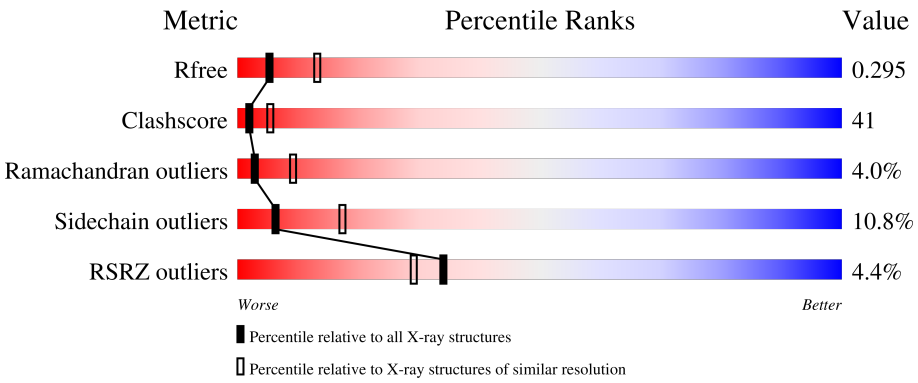
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 <=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	349	.% 39% 38% 8% 14%
1	B	349	.% 28% 34% 7% 32%
1	C	349	5% 30% 32% 6% • 32%
1	D	349	4% 27% 34% 7% • 32%
1	E	349	3% 33% 29% 7% 32%

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Mol	Chain	Length	Quality of chain
1	F	349	2% 28% 33% 7% 32%
1	G	349	5% 29% 30% 9% 32%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IMD	B	359	-	-	X	-
3	IMD	F	363	-	-	-	X
4	GOL	A	374	-	X	-	-
4	GOL	B	367	-	X	-	-
4	GOL	C	368	-	X	-	-
4	GOL	C	370	-	X	-	-
4	GOL	D	369	-	X	-	-
4	GOL	E	371	-	X	-	-
4	GOL	F	366	-	X	-	-
4	GOL	F	372	-	X	-	-
4	GOL	F	373	-	X	-	-

2 Entry composition (i)

There are 6 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 DNA repair and recombination protein rad51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	300	2317	1458	419	437	3	0	0	0
1	B	239	1879	1184	343	349	3	0	0	0
1	C	239	1879	1184	343	349	3	0	0	0
1	D	239	1879	1184	343	349	3	0	0	0
1	E	239	1879	1184	343	349	3	0	0	0
1	F	239	1879	1184	343	349	3	0	0	0
1	G	238	1875	1182	342	348	3	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP O74036
A	98	MSE	MET	MODIFIED RESIDUE	UNP O74036
A	154	MSE	MET	MODIFIED RESIDUE	UNP O74036
A	212	MSE	MET	MODIFIED RESIDUE	UNP O74036
B	1	MSE	MET	MODIFIED RESIDUE	UNP O74036
B	98	MSE	MET	MODIFIED RESIDUE	UNP O74036
B	154	MSE	MET	MODIFIED RESIDUE	UNP O74036
B	212	MSE	MET	MODIFIED RESIDUE	UNP O74036
C	1	MSE	MET	MODIFIED RESIDUE	UNP O74036
C	98	MSE	MET	MODIFIED RESIDUE	UNP O74036
C	154	MSE	MET	MODIFIED RESIDUE	UNP O74036
C	212	MSE	MET	MODIFIED RESIDUE	UNP O74036
D	1	MSE	MET	MODIFIED RESIDUE	UNP O74036
D	98	MSE	MET	MODIFIED RESIDUE	UNP O74036
D	154	MSE	MET	MODIFIED RESIDUE	UNP O74036

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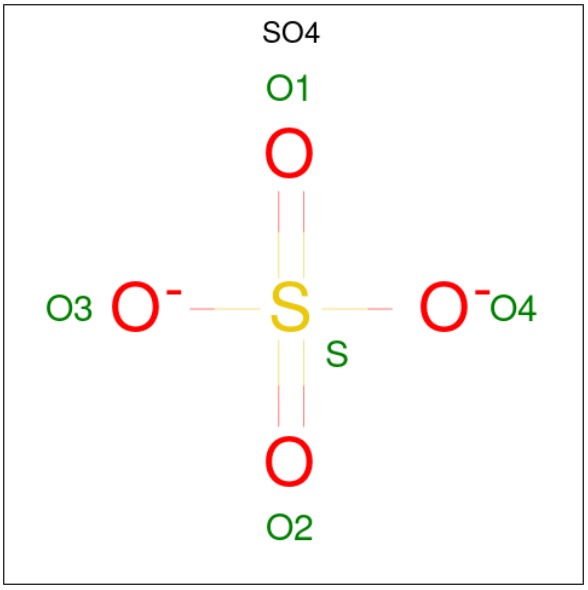
Chain	Residue	Modelled	Actual	Comment	Reference
D	212	MSE	MET	MODIFIED RESIDUE	UNP O74036
E	1	MSE	MET	MODIFIED RESIDUE	UNP O74036
E	98	MSE	MET	MODIFIED RESIDUE	UNP O74036
E	154	MSE	MET	MODIFIED RESIDUE	UNP O74036
E	212	MSE	MET	MODIFIED RESIDUE	UNP O74036
F	1	MSE	MET	MODIFIED RESIDUE	UNP O74036
F	98	MSE	MET	MODIFIED RESIDUE	UNP O74036
F	154	MSE	MET	MODIFIED RESIDUE	UNP O74036
F	212	MSE	MET	MODIFIED RESIDUE	UNP O74036
G	1	MSE	MET	MODIFIED RESIDUE	UNP O74036
G	98	MSE	MET	MODIFIED RESIDUE	UNP O74036
G	154	MSE	MET	MODIFIED RESIDUE	UNP O74036
G	212	MSE	MET	MODIFIED RESIDUE	UNP O74036

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	S		0	0
			5	4	1			
2	B	1	Total	O	S		0	0
			5	4	1			
2	C	1	Total	O	S		0	0
			5	4	1			
2	D	1	Total	O	S		0	0
			5	4	1			
2	E	1	Total	O	S		0	0
			5	4	1			

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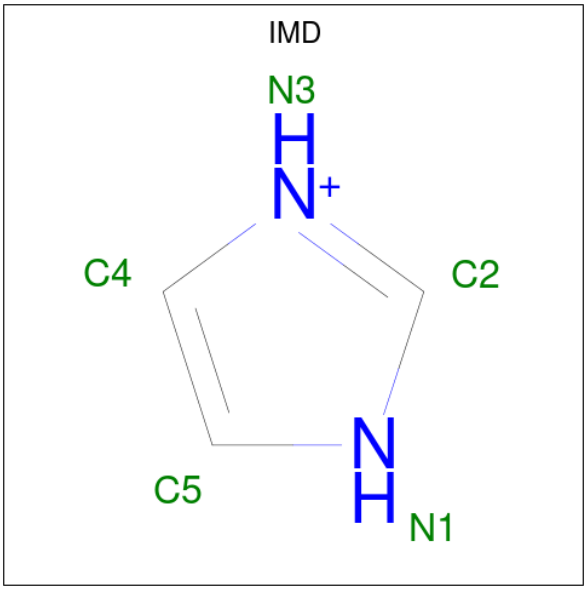
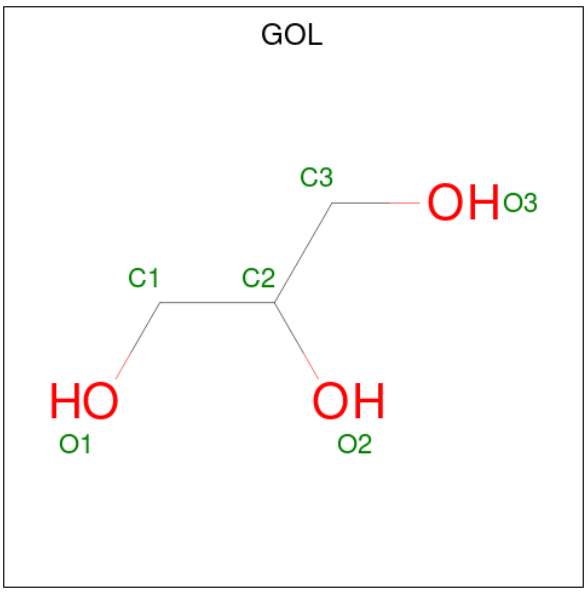
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	F	1	5	4	1	0	0
			Total	O	S		
2	G	1	5	4	1	0	0

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



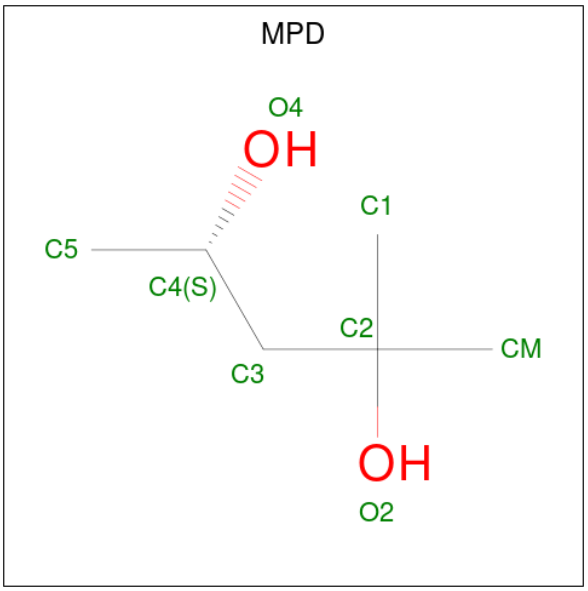
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	5	3	2	0	0
			Total	C	N		
3	A	1	5	3	2	0	0
			Total	C	N		
3	A	1	5	3	2	0	0
			Total	C	N		
3	A	1	5	3	2	0	0
			Total	C	N		
3	B	1	5	3	2	0	0
			Total	C	N		
3	B	1	5	3	2	0	0
			Total	C	N		
3	B	1	5	3	2	0	0
			Total	C	N		
3	C	1	5	3	2	0	0
			Total	C	N		
3	F	1	5	3	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			6	3	3			
4	B	1	Total	C	O		0	0
			6	3	3			
4	C	1	Total	C	O		0	0
			6	3	3			
4	C	1	Total	C	O		0	0
			6	3	3			
4	D	1	Total	C	O		0	0
			6	3	3			
4	E	1	Total	C	O		0	0
			6	3	3			
4	F	1	Total	C	O		0	0
			6	3	3			
4	F	1	Total	C	O		0	0
			6	3	3			
4	F	1	Total	C	O		0	0
			6	3	3			

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	8	6	2	0	0
5	E	1	8	6	2	0	0
5	G	1	8	6	2	0	0
5	G	1	8	6	2	0	0

- Molecule 6 is water.

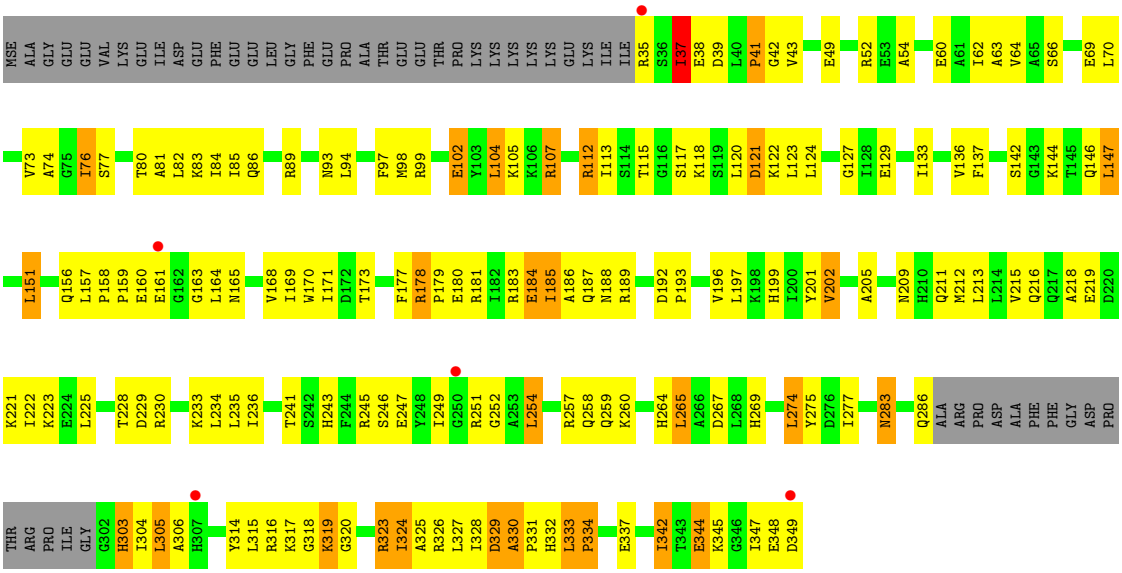
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	20	20	20	0	0
6	B	6	6	6	0	0
6	C	7	7	7	0	0
6	D	11	11	11	0	0
6	E	10	10	10	0	0
6	F	6	6	6	0	0
6	G	7	7	7	0	0

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.

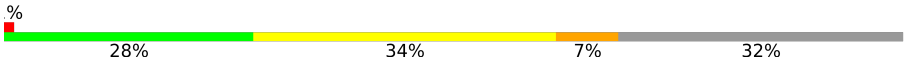
• Molecule 1: DNA repair and recombination protein rad51

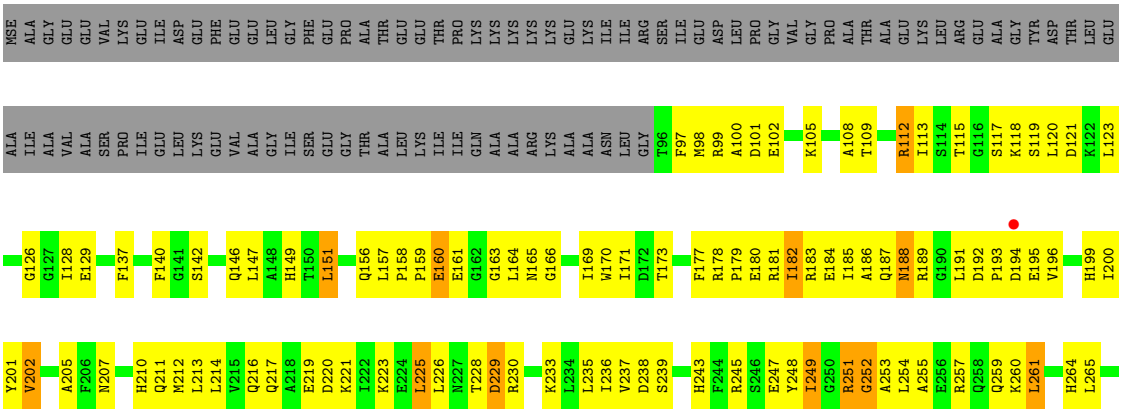
Chain A:

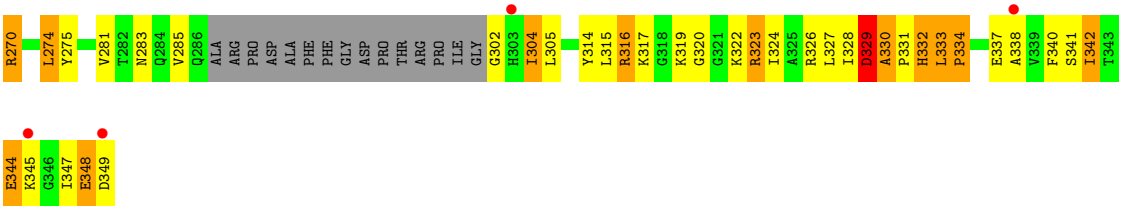


• Molecule 1: DNA repair and recombination protein rad51

Chain B:

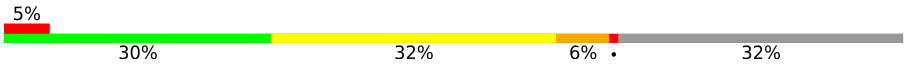


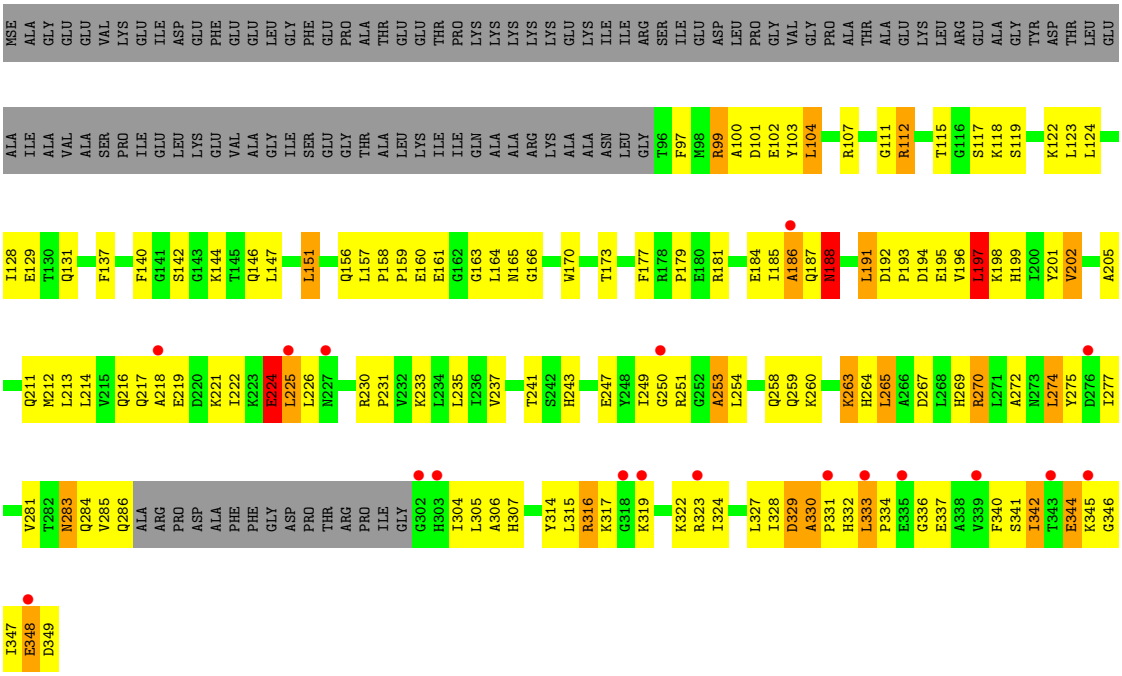




• Molecule 1: DNA repair and recombination protein rad51

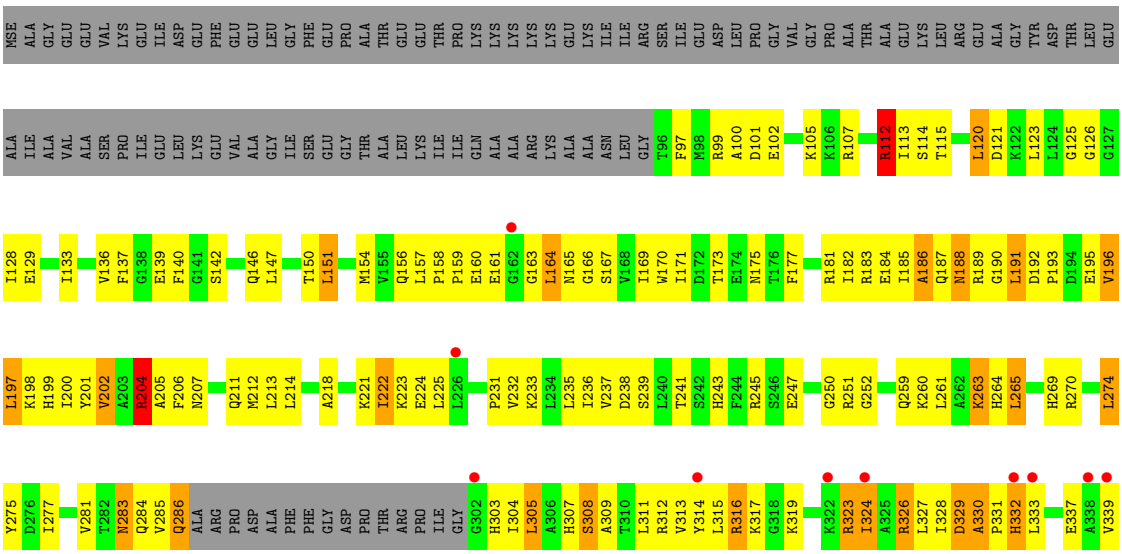
Chain C:

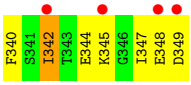




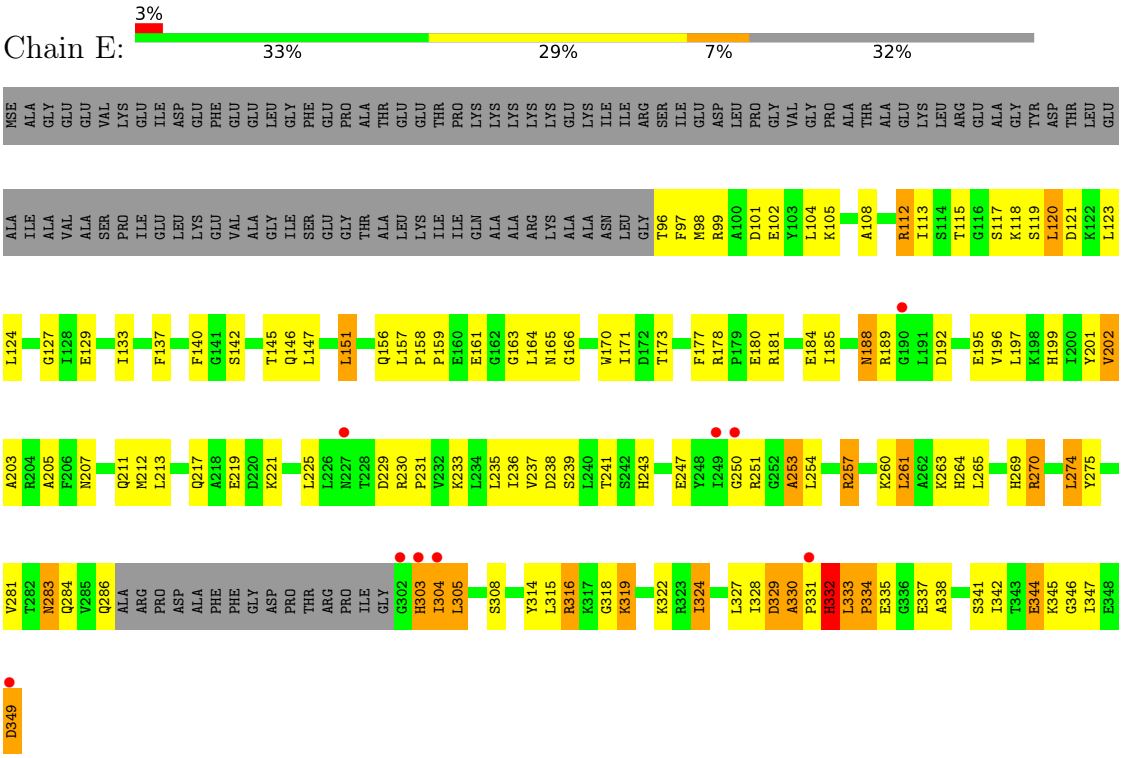
• Molecule 1: DNA repair and recombination protein rad51

Chain D:

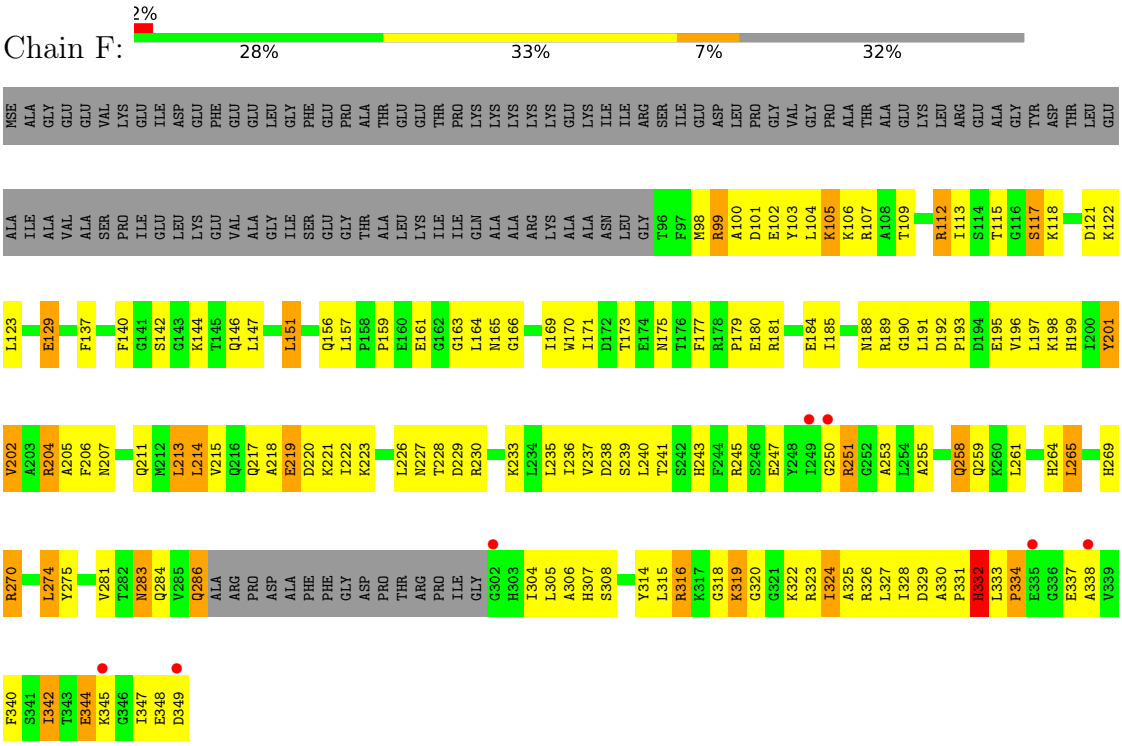




• Molecule 1: DNA repair and recombination protein rad51

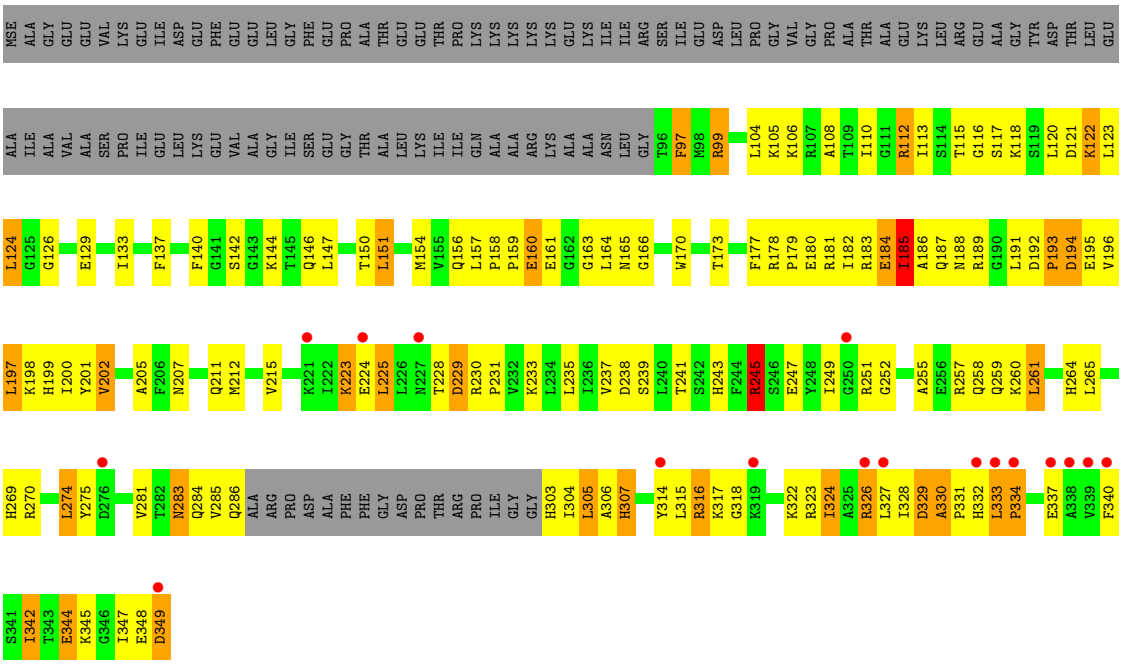


• Molecule 1: DNA repair and recombination protein rad51



• Molecule 1: DNA repair and recombination protein rad51

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	144.16Å 193.12Å 176.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.12 – 2.85 39.12 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.3 (39.12-2.85) 93.6 (39.12-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.307 0.245 , 0.295	Depositor DCC
R_{free} test set	5206 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 77.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13820	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, MPD, IMD

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	0.44	0/2347	0.78	8/3159 (0.3%)
1	B	0.41	0/1905	0.75	7/2560 (0.3%)
1	C	0.40	0/1905	0.76	7/2560 (0.3%)
1	D	0.40	0/1905	0.77	8/2560 (0.3%)
1	E	0.48	0/1905	0.77	6/2560 (0.2%)
1	F	0.45	0/1905	0.78	8/2560 (0.3%)
1	G	0.42	0/1901	0.86	10/2555 (0.4%)
All	All	0.43	0/13773	0.79	54/18514 (0.3%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	245	ARG	NE-CZ-NH2	-13.27	113.67	120.30
1	G	245	ARG	NE-CZ-NH1	12.99	126.80	120.30
1	A	178	ARG	NE-CZ-NH2	-12.62	113.99	120.30
1	A	178	ARG	NE-CZ-NH1	11.23	125.91	120.30
1	G	112	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	D	204	ARG	NE-CZ-NH2	9.16	124.88	120.30
1	F	204	ARG	NE-CZ-NH1	-9.16	115.72	120.30
1	F	270	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	B	112	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	D	204	ARG	NE-CZ-NH1	-8.99	115.80	120.30
1	B	112	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	F	204	ARG	NE-CZ-NH2	8.37	124.48	120.30
1	E	112	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	E	112	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	D	316	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	F	270	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	G	316	ARG	NE-CZ-NH1	-7.82	116.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	112	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	G	316	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	B	270	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	C	316	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	B	270	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	C	270	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	D	316	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	C	316	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	A	316	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	112	ARG	NE-CZ-NH1	-6.35	117.13	120.30
1	D	270	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	C	270	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	F	112	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	C	112	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	A	112	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	E	316	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	316	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	D	112	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	G	245	ARG	CD-NE-CZ	5.78	131.70	123.60
1	F	316	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	E	270	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	C	112	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	B	316	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	316	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	178	ARG	CD-NE-CZ	5.54	131.35	123.60
1	D	112	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	E	316	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	E	344	GLU	N-CA-C	-5.37	96.51	111.00
1	G	344	GLU	N-CA-C	-5.36	96.54	111.00
1	F	112	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	D	270	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	G	270	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	G	245	ARG	CG-CD-NE	-5.14	101.00	111.80
1	F	344	GLU	N-CA-C	-5.10	97.23	111.00
1	B	344	GLU	N-CA-C	-5.08	97.28	111.00
1	A	344	GLU	N-CA-C	-5.03	97.43	111.00
1	C	344	GLU	N-CA-C	-5.02	97.44	111.00

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	2317	0	2375	213	0
1	B	1879	0	1917	190	0
1	C	1879	0	1917	158	0
1	D	1879	0	1917	184	0
1	E	1879	0	1917	135	0
1	F	1879	0	1917	162	0
1	G	1875	0	1914	173	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	1	0
2	G	5	0	0	1	0
3	A	20	0	20	2	0
3	B	15	0	15	8	0
3	C	5	0	5	0	0
3	F	5	0	5	3	0
4	A	6	0	5	0	0
4	B	6	0	4	1	0
4	C	12	0	9	1	0
4	D	6	0	4	2	0
4	E	6	0	4	0	0
4	F	18	0	13	2	0
5	B	8	0	14	0	0
5	E	8	0	14	0	0
5	G	16	0	28	0	0
6	A	20	0	0	5	0
6	B	6	0	0	2	0
6	C	7	0	0	6	0
6	D	11	0	0	2	0
6	E	10	0	0	0	0
6	F	6	0	0	1	0
6	G	7	0	0	0	0
All	All	13820	0	14014	1144	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 41.

All (1144) 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)
4:D:369:GOL:C1	4:D:369:GOL:O1	1.64	1.46
4:F:373:GOL:C1	4:F:373:GOL:O1	1.65	1.42
1:F:324:ILE:HD11	1:F:337:GLU:HB3	1.28	1.11
1:A:317:LYS:HG3	1:A:323:ARG:HH12	0.98	1.10
1:B:324:ILE:HD11	1:B:337:GLU:HB3	1.34	1.09
1:E:330:ALA:H	1:E:331:PRO:HD2	1.15	1.06
1:B:228:THR:HG22	1:B:230:ARG:H	1.18	1.05
1:A:107:ARG:HH11	1:A:107:ARG:HB3	1.16	1.04
1:A:317:LYS:HG3	1:A:323:ARG:NH1	1.73	1.04
1:B:329:ASP:HB3	1:B:331:PRO:HD2	1.41	1.02
1:D:169:ILE:HG13	1:D:222:ILE:HD11	1.44	1.00
1:D:222:ILE:HD12	1:D:232:VAL:HG21	1.42	0.99
1:F:258:GLN:HE21	1:F:258:GLN:HA	1.27	0.98
1:D:183:ARG:HD2	1:D:193:PRO:HB2	1.45	0.97
1:E:156:GLN:NE2	1:E:196:VAL:HG13	1.79	0.97
1:A:330:ALA:H	1:A:331:PRO:HD2	1.30	0.96
1:C:251:ARG:HB3	1:D:251:ARG:HB2	1.48	0.96
1:G:317:LYS:HG3	1:G:323:ARG:HH12	1.29	0.96
1:D:187:GLN:HB3	1:D:193:PRO:HD3	1.44	0.96
1:C:107:ARG:HB3	1:C:107:ARG:HH11	1.30	0.95
1:A:246:SER:O	1:A:249:ILE:HD11	1.70	0.91
1:G:189:ARG:HH21	1:G:345:LYS:HB3	1.34	0.90
1:F:286:GLN:H	1:F:286:GLN:NE2	1.70	0.88
1:D:326:ARG:HH21	1:D:326:ARG:HB3	1.36	0.88
1:B:212:MSE:HE1	1:B:260:LYS:HD3	1.56	0.88
1:C:107:ARG:HB3	1:C:107:ARG:NH1	1.88	0.88
1:G:187:GLN:HB3	1:G:193:PRO:HB3	1.55	0.88
1:A:326:ARG:HD3	1:A:337:GLU:HG2	1.55	0.88
1:C:212:MSE:HE1	1:C:260:LYS:HD2	1.57	0.87
1:D:330:ALA:H	1:D:331:PRO:HD2	1.39	0.87
1:E:327:LEU:HD21	1:E:333:LEU:HD23	1.55	0.87
1:E:269:HIS:NE2	1:E:308:SER:HB3	1.89	0.86
1:E:157:LEU:HD13	1:E:161:GLU:HB2	1.57	0.86
1:A:249:ILE:HD12	1:A:249:ILE:N	1.90	0.86
1:B:330:ALA:H	1:B:331:PRO:HD2	1.37	0.86
1:A:157:LEU:HD13	1:A:161:GLU:CB	2.06	0.85
1:B:169:ILE:HD11	1:B:221:LYS:HG2	1.58	0.85
1:A:317:LYS:CG	1:A:323:ARG:HH12	1.86	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:LYS:HG3	1:D:323:ARG:HH12	1.42	0.85
1:C:330:ALA:H	1:C:331:PRO:HD2	1.40	0.85
1:A:37:ILE:HD11	1:A:52:ARG:HH12	1.42	0.85
1:G:115:THR:HG21	1:G:120:LEU:HD22	1.56	0.84
1:C:251:ARG:NH2	1:D:251:ARG:HA	1.93	0.83
1:D:261:LEU:HD22	1:D:304:ILE:HD11	1.60	0.83
1:C:185:ILE:HD12	1:C:346:GLY:N	1.94	0.83
1:F:228:THR:HG22	1:F:229:ASP:H	1.43	0.83
1:D:189:ARG:HH21	1:D:345:LYS:HB3	1.43	0.83
1:C:181:ARG:NH2	1:C:185:ILE:HD11	1.94	0.83
1:G:332:HIS:O	1:G:333:LEU:HB2	1.76	0.83
1:E:96:THR:HG22	1:E:97:PHE:H	1.43	0.83
1:F:340:PHE:HA	1:F:349:ASP:HB2	1.61	0.82
1:G:154:MSE:SE	1:G:189:ARG:HH11	2.11	0.82
1:F:228:THR:HG22	1:F:229:ASP:N	1.95	0.82
1:B:252:GLY:CA	3:B:359:IMD:HN3	1.92	0.82
1:A:252:GLY:H	1:G:251:ARG:NH2	1.77	0.82
1:G:181:ARG:O	1:G:185:ILE:HG22	1.80	0.81
1:F:245:ARG:HB3	1:F:304:ILE:HD11	1.62	0.81
1:A:212:MSE:HE1	1:A:260:LYS:HD3	1.61	0.81
1:B:304:ILE:HD13	1:B:305:LEU:N	1.94	0.81
1:A:252:GLY:H	1:G:251:ARG:HH22	1.28	0.81
1:C:157:LEU:HD13	1:C:161:GLU:HB2	1.63	0.81
1:C:251:ARG:HH21	1:D:251:ARG:HA	1.45	0.81
1:B:317:LYS:HG3	1:B:323:ARG:HH22	1.46	0.80
1:F:219:GLU:OE1	1:F:270:ARG:NH2	2.14	0.80
1:F:324:ILE:HD13	1:F:325:ALA:N	1.96	0.80
1:G:348:GLU:O	1:G:349:ASP:HB2	1.82	0.80
1:B:328:ILE:N	1:B:328:ILE:HD12	1.97	0.79
1:A:144:LYS:HG2	2:A:350:SO4:O1	1.82	0.79
1:F:258:GLN:HA	1:F:258:GLN:NE2	1.98	0.79
1:E:330:ALA:H	1:E:331:PRO:CD	1.93	0.78
1:A:80:THR:HA	1:A:83:LYS:HE2	1.63	0.78
1:D:285:VAL:O	1:D:286:GLN:HB3	1.82	0.78
1:C:173:THR:HG22	1:C:205:ALA:HB3	1.66	0.78
1:C:329:ASP:HB2	1:C:331:PRO:HD2	1.65	0.78
1:D:114:SER:HA	1:D:121:ASP:OD2	1.83	0.78
1:A:330:ALA:N	1:A:331:PRO:HD2	1.98	0.78
1:D:188:ASN:OD1	1:D:344:GLU:HB3	1.84	0.78
1:B:330:ALA:H	1:B:331:PRO:CD	1.98	0.77
1:A:107:ARG:HB3	1:A:107:ARG:NH1	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:HIS:CE1	1:E:178:ARG:HE	2.03	0.77
1:E:286:GLN:H	1:E:303:HIS:CE1	2.03	0.77
1:A:107:ARG:HH11	1:A:107:ARG:CB	1.96	0.77
1:A:157:LEU:HD13	1:A:161:GLU:HB3	1.67	0.77
1:G:163:GLY:O	1:G:164:LEU:HD22	1.85	0.76
1:F:173:THR:HG22	1:F:205:ALA:HB3	1.66	0.76
1:D:139:GLU:OE1	1:D:286:GLN:HG2	1.86	0.76
1:C:104:LEU:HD22	1:C:104:LEU:O	1.84	0.76
1:A:74:ALA:HB3	1:A:76:ILE:HD12	1.67	0.75
1:B:314:TYR:CB	1:B:328:ILE:HD11	2.16	0.75
1:C:187:GLN:HE21	1:C:193:PRO:HG3	1.49	0.75
1:A:38:GLU:HB2	6:A:430:HOH:O	1.86	0.75
1:A:221:LYS:HG3	1:A:225:LEU:HD13	1.68	0.75
1:B:252:GLY:HA2	3:B:359:IMD:HN3	1.50	0.75
1:B:146:GLN:HA	1:B:146:GLN:HE21	1.52	0.75
1:G:117:SER:HB3	1:G:347:ILE:HG22	1.69	0.75
1:A:332:HIS:O	1:A:333:LEU:HB2	1.85	0.75
1:A:324:ILE:CD1	1:A:337:GLU:HB3	2.17	0.74
1:D:156:GLN:NE2	1:D:196:VAL:HG12	2.02	0.74
1:G:113:ILE:HD13	1:G:164:LEU:HD23	1.70	0.74
1:G:317:LYS:HG3	1:G:323:ARG:NH1	2.02	0.74
1:C:99:ARG:HG2	1:C:101:ASP:OD2	1.87	0.74
1:A:199:HIS:HA	6:A:437:HOH:O	1.87	0.74
1:E:304:ILE:HG12	1:E:305:LEU:N	2.03	0.74
1:E:261:LEU:HG	1:E:304:ILE:HD11	1.69	0.73
1:G:225:LEU:HD11	1:G:230:ARG:O	1.86	0.73
1:D:186:ALA:HB1	1:D:196:VAL:HG21	1.70	0.73
1:D:311:LEU:HD11	1:D:327:LEU:HD22	1.71	0.73
1:F:241:THR:HB	1:F:304:ILE:HD12	1.70	0.73
1:E:173:THR:HG22	1:E:205:ALA:HB3	1.71	0.73
1:C:170:TRP:HB3	1:C:202:VAL:HG12	1.71	0.73
1:A:37:ILE:CG1	1:A:38:GLU:H	2.02	0.73
1:B:163:GLY:O	1:B:164:LEU:HD23	1.89	0.73
1:B:157:LEU:HD13	1:B:161:GLU:CB	2.19	0.72
1:G:157:LEU:HD13	1:G:161:GLU:HB2	1.71	0.72
1:G:185:ILE:HA	1:G:345:LYS:H	1.52	0.72
1:C:194:ASP:O	1:C:198:LYS:HE3	1.88	0.72
1:B:328:ILE:HD12	1:B:328:ILE:H	1.53	0.72
1:C:187:GLN:HB3	1:C:193:PRO:HD3	1.72	0.72
1:G:187:GLN:HB3	1:G:193:PRO:CB	2.18	0.72
1:C:146:GLN:HA	1:C:146:GLN:HE21	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:GLN:NE2	1:G:196:VAL:HG13	2.04	0.72
1:A:160:GLU:CD	1:A:160:GLU:H	1.91	0.71
1:D:157:LEU:HD13	1:D:161:GLU:HB2	1.70	0.71
1:D:182:ILE:HD13	1:D:200:ILE:HD12	1.71	0.71
1:C:163:GLY:O	1:C:164:LEU:HD23	1.90	0.71
1:G:118:LYS:HB2	1:G:349:ASP:O	1.89	0.71
1:A:252:GLY:N	1:G:251:ARG:HH22	1.87	0.71
1:A:330:ALA:H	1:A:331:PRO:CD	2.03	0.71
1:C:156:GLN:NE2	1:C:196:VAL:HG13	2.04	0.71
1:E:146:GLN:HE21	1:E:146:GLN:HA	1.55	0.71
1:G:316:ARG:NH1	1:G:324:ILE:HD12	2.06	0.71
1:B:123:LEU:HD12	1:B:334:PRO:HG2	1.71	0.70
1:B:158:PRO:HD2	1:B:161:GLU:HG3	1.73	0.70
1:F:103:TYR:O	1:F:107:ARG:HG3	1.92	0.70
1:B:323:ARG:HE	1:B:342:ILE:HG13	1.57	0.70
1:D:332:HIS:C	1:D:333:LEU:HD22	2.12	0.70
1:F:304:ILE:HG22	1:F:305:LEU:H	1.56	0.70
1:C:181:ARG:HH22	1:C:185:ILE:HD11	1.55	0.70
1:B:118:LYS:H	1:B:349:ASP:HB2	1.54	0.70
1:A:63:ALA:O	1:A:89:ARG:HD3	1.91	0.70
1:F:146:GLN:HE21	1:F:146:GLN:HA	1.56	0.70
1:A:328:ILE:HG22	1:A:328:ILE:O	1.91	0.70
1:C:170:TRP:HB3	1:C:202:VAL:CG1	2.22	0.70
1:C:330:ALA:N	1:C:331:PRO:HD2	2.06	0.70
1:C:331:PRO:O	1:C:332:HIS:HB2	1.90	0.70
1:G:324:ILE:HD13	1:G:324:ILE:C	2.12	0.70
1:D:115:THR:HG21	1:D:120:LEU:HD12	1.72	0.70
1:G:185:ILE:HG13	1:G:345:LYS:HA	1.72	0.69
1:A:156:GLN:NE2	1:A:196:VAL:HG13	2.07	0.69
1:B:170:TRP:HB3	1:B:202:VAL:HG12	1.73	0.69
1:G:187:GLN:HE21	1:G:193:PRO:HG3	1.58	0.69
1:D:146:GLN:HE21	1:D:146:GLN:HA	1.57	0.69
1:E:230:ARG:HB3	1:E:230:ARG:NH1	2.08	0.69
1:E:328:ILE:O	1:E:329:ASP:HB3	1.91	0.69
1:A:251:ARG:HE	1:B:251:ARG:NH2	1.91	0.69
1:A:258:GLN:HG3	1:B:249:ILE:CD1	2.22	0.69
1:E:157:LEU:HD13	1:E:161:GLU:CB	2.23	0.69
1:E:177:PHE:CD2	1:E:202:VAL:HG11	2.28	0.69
1:G:185:ILE:HG13	1:G:345:LYS:CA	2.23	0.69
1:F:221:LYS:NZ	3:F:363:IMD:H4	2.07	0.69
1:B:324:ILE:HD11	1:B:337:GLU:CB	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:LEU:HB3	1:B:334:PRO:HD2	1.75	0.68
1:G:146:GLN:HE21	1:G:146:GLN:HA	1.57	0.68
1:D:317:LYS:HG3	1:D:323:ARG:NH1	2.07	0.68
1:E:221:LYS:HE3	1:E:225:LEU:HD11	1.74	0.68
1:E:274:LEU:HD12	1:E:275:TYR:CZ	2.29	0.68
1:B:157:LEU:HD13	1:B:161:GLU:HB2	1.75	0.68
1:C:187:GLN:NE2	1:C:193:PRO:HG3	2.09	0.68
1:E:124:LEU:HA	1:E:333:LEU:HD21	1.75	0.68
1:A:249:ILE:HD13	1:G:258:GLN:HG3	1.75	0.68
1:D:330:ALA:N	1:D:331:PRO:HD2	2.08	0.68
1:D:159:PRO:HD3	1:D:165:ASN:ND2	2.09	0.68
1:F:142:SER:O	1:F:323:ARG:HD2	1.94	0.68
1:G:189:ARG:NH2	1:G:345:LYS:HB3	2.08	0.68
1:B:213:LEU:HG	1:B:217:GLN:OE1	1.94	0.67
1:B:317:LYS:HG3	1:B:323:ARG:NH2	2.08	0.67
1:C:159:PRO:HD3	1:C:165:ASN:ND2	2.08	0.67
1:C:304:ILE:HG12	1:C:305:LEU:N	2.09	0.67
1:D:173:THR:HG22	1:D:205:ALA:HB3	1.75	0.67
1:B:146:GLN:HE22	1:B:181:ARG:HE	1.42	0.67
1:F:326:ARG:HD3	1:F:337:GLU:HG2	1.76	0.67
1:F:113:ILE:HD11	1:F:164:LEU:HD12	1.75	0.67
1:A:344:GLU:H	1:A:344:GLU:CD	1.98	0.67
1:B:173:THR:HG22	1:B:205:ALA:HB3	1.77	0.67
1:F:228:THR:CG2	1:F:229:ASP:H	2.06	0.67
1:E:327:LEU:C	1:E:328:ILE:HD12	2.15	0.67
1:C:107:ARG:HH11	1:C:107:ARG:CB	2.06	0.67
1:C:188:ASN:ND2	1:C:188:ASN:O	2.26	0.67
1:C:181:ARG:HH22	1:C:185:ILE:CD1	2.08	0.67
1:E:96:THR:HG22	1:E:97:PHE:N	2.10	0.67
1:G:229:ASP:OD2	1:G:229:ASP:N	2.28	0.67
1:C:225:LEU:HB3	1:C:231:PRO:HA	1.76	0.66
1:A:74:ALA:HB3	1:A:76:ILE:CD1	2.25	0.66
1:A:324:ILE:HD11	1:A:337:GLU:HB3	1.76	0.66
1:G:182:ILE:HB	1:G:197:LEU:HD21	1.76	0.66
1:C:177:PHE:CD2	1:C:202:VAL:HG11	2.31	0.66
1:E:261:LEU:HD13	1:E:261:LEU:C	2.15	0.66
1:E:189:ARG:HE	1:E:345:LYS:HB3	1.61	0.66
1:E:328:ILE:O	1:E:328:ILE:HG22	1.95	0.66
1:B:330:ALA:N	1:B:331:PRO:CD	2.59	0.66
1:G:159:PRO:HD3	1:G:165:ASN:ND2	2.10	0.66
1:D:327:LEU:HD13	1:D:333:LEU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:MSE:SE	1:G:189:ARG:NH1	2.79	0.65
1:D:177:PHE:CD2	1:D:202:VAL:HG11	2.30	0.65
1:F:274:LEU:HD12	1:F:275:TYR:CZ	2.31	0.65
1:D:222:ILE:HG21	1:D:277:ILE:HD11	1.78	0.65
1:F:189:ARG:HH21	1:F:189:ARG:HG3	1.61	0.65
1:G:177:PHE:CD2	1:G:202:VAL:HG11	2.32	0.65
1:F:213:LEU:O	1:F:217:GLN:HG3	1.96	0.65
1:B:192:ASP:OD2	1:B:195:GLU:HB2	1.96	0.65
1:F:327:LEU:O	1:F:328:ILE:HD13	1.97	0.65
1:B:274:LEU:HD12	1:B:275:TYR:CZ	2.32	0.65
1:D:160:GLU:CD	1:D:160:GLU:H	1.99	0.65
1:D:328:ILE:O	1:D:328:ILE:HG22	1.96	0.65
1:F:171:ILE:HG23	1:F:214:LEU:HD23	1.77	0.65
1:D:189:ARG:HB3	1:D:345:LYS:HG2	1.77	0.65
1:G:170:TRP:HB3	1:G:202:VAL:HG12	1.79	0.65
1:G:344:GLU:CD	1:G:344:GLU:H	1.99	0.64
1:B:170:TRP:HB3	1:B:202:VAL:CG1	2.27	0.64
1:C:225:LEU:H	1:C:225:LEU:HD22	1.62	0.64
1:D:189:ARG:HE	1:D:345:LYS:HB3	1.63	0.64
1:A:37:ILE:CD1	1:A:38:GLU:H	2.11	0.64
1:C:251:ARG:CB	1:D:251:ARG:HB2	2.25	0.64
1:F:156:GLN:NE2	1:F:196:VAL:HG13	2.13	0.64
1:A:178:ARG:HH11	1:G:332:HIS:CD2	2.15	0.64
1:B:219:GLU:CD	1:B:270:ARG:HH22	2.01	0.64
1:B:344:GLU:CD	1:B:344:GLU:H	2.01	0.64
1:F:255:ALA:O	1:F:259:GLN:HB2	1.97	0.64
1:G:228:THR:HG23	1:G:229:ASP:OD2	1.98	0.64
1:A:173:THR:HG22	1:A:205:ALA:HB3	1.80	0.64
1:B:324:ILE:HD12	1:B:338:ALA:O	1.98	0.64
1:A:37:ILE:HD13	1:A:38:GLU:H	1.63	0.63
4:F:373:GOL:C1	4:F:373:GOL:HO1	2.09	0.63
1:A:254:LEU:HD22	1:B:249:ILE:HD11	1.80	0.63
1:G:188:ASN:O	1:G:345:LYS:HE2	1.98	0.63
1:F:146:GLN:HA	1:F:146:GLN:NE2	2.13	0.63
1:B:257:ARG:O	1:B:261:LEU:HB2	1.98	0.63
1:D:186:ALA:CB	1:D:196:VAL:HG21	2.28	0.63
1:F:251:ARG:N	1:F:251:ARG:HD3	2.11	0.63
1:A:69:GLU:O	1:A:73:VAL:HG23	1.99	0.63
1:C:317:LYS:HG3	1:C:323:ARG:HH12	1.64	0.63
1:D:327:LEU:C	1:D:328:ILE:HD12	2.19	0.63
1:F:190:GLY:O	1:F:191:LEU:HD23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLN:HE21	1:A:146:GLN:HA	1.63	0.63
1:C:344:GLU:H	1:C:344:GLU:CD	2.02	0.63
1:F:177:PHE:CD2	1:F:202:VAL:HG11	2.34	0.63
1:E:304:ILE:HG12	1:E:305:LEU:H	1.63	0.63
1:G:187:GLN:HB3	1:G:193:PRO:CG	2.29	0.63
1:G:327:LEU:HD12	1:G:327:LEU:N	2.14	0.63
1:A:211:GLN:HE21	1:A:264:HIS:CE1	2.17	0.62
1:F:328:ILE:O	1:F:328:ILE:HG22	1.98	0.62
1:G:330:ALA:HB3	1:G:331:PRO:HD3	1.81	0.62
1:C:317:LYS:HG3	1:C:323:ARG:NH1	2.13	0.62
1:F:99:ARG:HB3	1:F:102:GLU:HG2	1.80	0.62
1:F:344:GLU:H	1:F:344:GLU:CD	2.03	0.62
1:A:259:GLN:NE2	1:B:247:GLU:HB3	2.15	0.62
1:G:170:TRP:HB3	1:G:202:VAL:CG1	2.29	0.62
1:A:188:ASN:ND2	1:A:344:GLU:CB	2.63	0.62
1:B:146:GLN:HA	1:B:146:GLN:NE2	2.14	0.62
1:D:189:ARG:NH2	1:D:345:LYS:HB3	2.13	0.62
1:E:146:GLN:HA	1:E:146:GLN:NE2	2.14	0.62
1:E:146:GLN:HE22	1:E:181:ARG:HE	1.48	0.62
1:A:37:ILE:CD1	1:A:52:ARG:HH12	2.13	0.62
1:C:218:ALA:O	1:C:222:ILE:HG13	1.99	0.62
1:F:146:GLN:HE22	1:F:181:ARG:HE	1.46	0.62
1:F:101:ASP:OD2	1:F:102:GLU:N	2.33	0.62
1:G:144:LYS:HG2	2:G:356:SO4:O2	1.99	0.61
1:A:170:TRP:HB3	1:A:202:VAL:HG12	1.82	0.61
1:C:181:ARG:O	1:C:185:ILE:HG12	2.00	0.61
1:G:327:LEU:HD12	1:G:327:LEU:H	1.65	0.61
1:A:171:ILE:CD1	1:G:97:PHE:HE1	2.13	0.61
1:A:219:GLU:O	1:A:223:LYS:HG2	2.00	0.61
1:D:190:GLY:O	1:D:191:LEU:HB2	2.01	0.61
1:D:222:ILE:HD13	1:D:222:ILE:N	2.16	0.61
1:E:137:PHE:CZ	1:E:314:TYR:HB2	2.35	0.61
1:E:330:ALA:N	1:E:331:PRO:HD2	1.98	0.61
1:G:228:THR:HG22	1:G:230:ARG:H	1.65	0.61
1:C:118:LYS:HB2	1:C:349:ASP:OD1	1.99	0.61
1:C:156:GLN:OE1	1:C:199:HIS:HB2	2.01	0.61
1:A:159:PRO:HD3	1:A:165:ASN:ND2	2.15	0.61
1:E:96:THR:HG22	1:E:97:PHE:HD1	1.65	0.61
1:A:157:LEU:HD13	1:A:161:GLU:HB2	1.80	0.61
1:D:185:ILE:HG23	1:D:345:LYS:HA	1.82	0.61
1:G:173:THR:HG22	1:G:205:ALA:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:PHE:CD2	1:A:202:VAL:HG11	2.35	0.61
1:A:252:GLY:CA	1:G:251:ARG:HH22	2.13	0.61
1:A:251:ARG:HG3	1:A:251:ARG:HH11	1.65	0.61
1:E:344:GLU:O	1:E:345:LYS:HB2	2.00	0.61
1:A:178:ARG:HD2	1:G:332:HIS:NE2	2.16	0.60
1:D:274:LEU:HD12	1:D:275:TYR:CZ	2.36	0.60
1:B:183:ARG:HG3	1:B:193:PRO:HB2	1.83	0.60
1:C:146:GLN:HA	1:C:146:GLN:NE2	2.16	0.60
1:E:119:SER:HB2	1:E:349:ASP:OD1	2.01	0.60
1:F:98:MSE:CG	1:F:102:GLU:HB2	2.31	0.60
1:G:274:LEU:HD12	1:G:275:TYR:CZ	2.36	0.60
1:A:331:PRO:HD3	1:B:140:PHE:HZ	1.67	0.60
1:E:257:ARG:NH2	1:E:304:ILE:HB	2.17	0.60
1:F:105:LYS:HG3	1:F:106:LYS:N	2.16	0.60
1:C:274:LEU:HD12	1:C:275:TYR:CZ	2.37	0.60
1:D:344:GLU:CD	1:D:344:GLU:H	2.04	0.60
1:E:333:LEU:HG	1:E:334:PRO:HD2	1.84	0.60
1:G:113:ILE:CD1	1:G:164:LEU:HD23	2.32	0.60
1:G:274:LEU:HD13	1:G:274:LEU:O	2.01	0.60
1:G:328:ILE:N	1:G:328:ILE:HD12	2.16	0.60
1:A:113:ILE:CD1	1:A:164:LEU:HG	2.32	0.60
1:E:201:TYR:CD2	1:E:221:LYS:HE2	2.37	0.60
1:E:344:GLU:CD	1:E:344:GLU:H	2.05	0.60
1:C:111:GLY:HA3	6:C:404:HOH:O	2.00	0.60
1:D:330:ALA:H	1:D:331:PRO:CD	2.10	0.59
1:F:215:VAL:HG21	1:F:264:HIS:NE2	2.16	0.59
1:D:263:LYS:NZ	1:D:263:LYS:HB3	2.17	0.59
1:D:329:ASP:CG	1:D:330:ALA:H	2.02	0.59
1:A:221:LYS:O	1:A:225:LEU:HD13	2.02	0.59
1:D:223:LYS:HB2	1:D:223:LYS:NZ	2.17	0.59
1:C:251:ARG:HA	1:C:254:LEU:HB3	1.84	0.59
1:D:225:LEU:HD12	1:D:225:LEU:N	2.17	0.59
1:D:326:ARG:HG2	1:D:327:LEU:N	2.18	0.59
1:A:42:GLY:HA3	1:A:84:ILE:HD11	1.85	0.59
1:B:255:ALA:O	1:B:259:GLN:HG2	2.02	0.59
1:F:332:HIS:CE1	1:G:178:ARG:HH11	2.19	0.59
1:B:316:ARG:HH12	1:B:326:ARG:HH21	1.49	0.59
1:E:146:GLN:HG3	1:E:342:ILE:HD12	1.84	0.59
1:G:146:GLN:HA	1:G:146:GLN:NE2	2.17	0.59
1:D:121:ASP:O	1:D:126:GLY:N	2.32	0.59
1:E:257:ARG:CZ	1:E:304:ILE:HB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:VAL:C	1:G:198:LYS:H	2.05	0.59
1:A:228:THR:HG22	1:A:229:ASP:N	2.18	0.59
1:A:317:LYS:HE2	1:A:323:ARG:HH22	1.68	0.58
1:B:228:THR:HG22	1:B:230:ARG:N	2.02	0.58
1:C:117:SER:HB3	1:C:347:ILE:HG22	1.85	0.58
1:D:146:GLN:HA	1:D:146:GLN:NE2	2.16	0.58
1:E:185:ILE:HG12	1:E:346:GLY:N	2.18	0.58
1:E:328:ILE:O	1:E:329:ASP:CB	2.51	0.58
1:G:223:LYS:O	1:G:225:LEU:N	2.35	0.58
1:C:285:VAL:O	1:C:286:GLN:CB	2.51	0.58
1:D:326:ARG:HB3	1:D:326:ARG:NH2	2.13	0.58
1:B:100:ALA:HB1	1:C:197:LEU:HD13	1.85	0.58
1:D:344:GLU:O	1:D:345:LYS:HB2	2.03	0.58
1:F:98:MSE:HG2	1:F:102:GLU:HB2	1.85	0.58
1:B:177:PHE:HE1	1:B:182:ILE:HD12	1.69	0.58
1:E:184:GLU:O	1:E:188:ASN:HB2	2.03	0.58
1:B:314:TYR:N	1:B:328:ILE:HD11	2.19	0.58
1:F:170:TRP:HB3	1:F:202:VAL:CG1	2.33	0.58
1:G:112:ARG:HD3	1:G:126:GLY:HA3	1.86	0.58
1:C:213:LEU:O	1:C:213:LEU:HD23	2.04	0.58
1:D:113:ILE:HD11	1:D:164:LEU:HD12	1.84	0.58
1:B:184:GLU:HG2	6:B:386:HOH:O	2.03	0.58
1:D:303:HIS:HE1	1:D:305:LEU:HD13	1.69	0.58
1:B:156:GLN:OE1	1:B:199:HIS:HB2	2.04	0.58
1:G:156:GLN:OE1	1:G:199:HIS:HB2	2.04	0.58
1:A:258:GLN:HG3	1:B:249:ILE:HD12	1.83	0.58
1:B:314:TYR:HB2	1:B:328:ILE:HD11	1.86	0.58
1:C:185:ILE:HA	6:C:384:HOH:O	2.04	0.58
1:F:104:LEU:HD12	1:G:180:GLU:HG3	1.85	0.58
1:B:159:PRO:HD3	1:B:165:ASN:ND2	2.19	0.57
1:E:213:LEU:HD22	1:E:213:LEU:O	2.04	0.57
1:F:251:ARG:C	1:F:253:ALA:H	2.07	0.57
1:B:187:GLN:HG3	1:B:188:ASN:N	2.18	0.57
1:E:225:LEU:N	1:E:225:LEU:HD12	2.19	0.57
1:A:344:GLU:O	1:A:345:LYS:HB2	2.05	0.57
1:B:99:ARG:HE	1:C:198:LYS:HA	1.67	0.57
1:C:191:LEU:N	1:C:191:LEU:HD12	2.19	0.57
1:E:159:PRO:HD3	1:E:165:ASN:ND2	2.18	0.57
1:A:328:ILE:O	1:A:329:ASP:HB3	2.04	0.57
1:F:137:PHE:CZ	1:F:314:TYR:HB2	2.39	0.57
1:A:330:ALA:N	1:A:331:PRO:CD	2.65	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ARG:NH1	1:B:326:ARG:HH21	2.02	0.57
1:C:181:ARG:NH2	1:C:185:ILE:CD1	2.65	0.57
1:D:154:MSE:SE	1:D:189:ARG:HH11	2.38	0.57
1:E:322:LYS:NZ	1:E:341:SER:HB3	2.18	0.57
1:D:177:PHE:CE1	1:D:182:ILE:HD11	2.38	0.57
1:A:37:ILE:HD11	1:A:52:ARG:NH1	2.17	0.57
1:B:332:HIS:HB3	1:B:333:LEU:HD12	1.86	0.57
1:C:99:ARG:HH22	4:C:368:GOL:H12	1.69	0.57
1:D:139:GLU:HG2	1:D:286:GLN:HB3	1.86	0.57
1:C:226:LEU:HA	1:C:231:PRO:HB3	1.87	0.57
1:D:170:TRP:HB3	1:D:202:VAL:CG1	2.34	0.57
1:A:211:GLN:HE21	1:A:264:HIS:HE1	1.51	0.57
1:B:323:ARG:HH21	1:B:323:ARG:HG3	1.69	0.57
1:D:329:ASP:CG	1:D:330:ALA:N	2.57	0.57
1:A:320:GLY:HA2	3:A:361:IMD:N3	2.20	0.56
1:D:146:GLN:HG3	1:D:342:ILE:HD12	1.87	0.56
1:D:332:HIS:O	1:D:333:LEU:HD22	2.05	0.56
1:F:170:TRP:HB3	1:F:202:VAL:HG12	1.86	0.56
1:A:37:ILE:HG12	1:A:38:GLU:H	1.69	0.56
1:A:274:LEU:HD12	1:A:275:TYR:CZ	2.40	0.56
1:B:187:GLN:C	1:B:189:ARG:H	2.09	0.56
1:A:123:LEU:HG	1:A:327:LEU:HD13	1.86	0.56
1:A:213:LEU:O	1:A:216:GLN:HG2	2.05	0.56
1:A:274:LEU:HD13	1:A:274:LEU:O	2.04	0.56
1:F:157:LEU:HD13	1:F:161:GLU:CB	2.34	0.56
1:G:329:ASP:O	1:G:330:ALA:HB2	2.05	0.56
1:D:156:GLN:OE1	1:D:199:HIS:HB2	2.05	0.56
4:D:369:GOL:C1	4:D:369:GOL:HO1	2.08	0.56
1:B:322:LYS:NZ	1:B:341:SER:HB3	2.20	0.56
1:C:286:GLN:HE21	1:C:286:GLN:HA	1.70	0.56
1:F:169:ILE:HD11	1:F:221:LYS:CG	2.35	0.56
1:F:228:THR:HG22	1:F:230:ARG:H	1.70	0.56
1:E:333:LEU:CG	1:E:334:PRO:HD2	2.36	0.56
1:F:228:THR:CG2	1:F:229:ASP:N	2.62	0.56
1:E:344:GLU:O	1:E:345:LYS:CB	2.54	0.56
1:B:149:HIS:HD2	1:B:182:ILE:HG13	1.70	0.56
1:G:97:PHE:N	1:G:97:PHE:CD2	2.72	0.56
1:G:211:GLN:HE21	1:G:264:HIS:CE1	2.24	0.56
1:A:188:ASN:ND2	1:A:344:GLU:HB3	2.21	0.56
1:D:190:GLY:O	1:D:191:LEU:CB	2.53	0.56
1:F:159:PRO:HD3	1:F:165:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ASN:OD1	1:C:344:GLU:HB3	2.06	0.56
1:G:344:GLU:O	1:G:345:LYS:HB2	2.05	0.56
1:A:163:GLY:O	1:A:164:LEU:HD23	2.04	0.55
1:A:286:GLN:HA	1:A:286:GLN:NE2	2.20	0.55
1:B:211:GLN:HE21	1:B:264:HIS:HE1	1.54	0.55
1:F:175:ASN:H	1:F:204:ARG:NH1	2.03	0.55
1:A:147:LEU:HD22	1:A:151:LEU:HD22	1.88	0.55
1:B:211:GLN:HE21	1:B:264:HIS:CE1	2.24	0.55
1:E:98:MSE:HG3	1:E:102:GLU:OE1	2.06	0.55
1:E:322:LYS:HZ2	1:E:341:SER:HB3	1.71	0.55
1:D:187:GLN:HB3	1:D:193:PRO:CD	2.28	0.55
1:G:314:TYR:HB3	1:G:328:ILE:HD11	1.89	0.55
1:A:37:ILE:CG1	1:A:38:GLU:N	2.69	0.55
1:A:81:ALA:O	1:A:85:ILE:HG12	2.06	0.55
1:B:177:PHE:CD2	1:B:202:VAL:HG11	2.42	0.55
1:D:326:ARG:HH21	1:D:326:ARG:CB	2.12	0.55
1:E:324:ILE:HD11	1:E:337:GLU:HB3	1.89	0.55
1:F:286:GLN:H	1:F:286:GLN:CD	2.09	0.55
1:F:330:ALA:N	1:F:331:PRO:HD2	2.21	0.55
1:A:82:LEU:HD13	1:A:82:LEU:C	2.27	0.55
1:B:344:GLU:O	1:B:345:LYS:HB2	2.07	0.55
1:A:171:ILE:HD11	1:G:97:PHE:HE1	1.71	0.55
1:C:196:VAL:C	1:C:198:LYS:H	2.09	0.55
1:D:183:ARG:C	1:D:185:ILE:H	2.10	0.55
1:E:274:LEU:HD13	1:E:274:LEU:O	2.06	0.55
1:F:344:GLU:O	1:F:345:LYS:HB2	2.05	0.55
1:D:330:ALA:N	1:D:331:PRO:CD	2.68	0.55
1:E:156:GLN:HE22	1:E:196:VAL:HG13	1.68	0.55
1:G:225:LEU:HG	1:G:231:PRO:HA	1.89	0.55
1:D:332:HIS:ND1	6:D:399:HOH:O	2.34	0.54
1:F:274:LEU:HD13	1:F:274:LEU:O	2.07	0.54
1:A:118:LYS:O	1:A:122:LYS:HG3	2.07	0.54
1:A:286:GLN:HA	1:A:286:GLN:HE21	1.72	0.54
1:D:225:LEU:O	1:D:231:PRO:HA	2.06	0.54
1:G:245:ARG:O	1:G:245:ARG:HG3	2.08	0.54
1:C:344:GLU:O	1:C:345:LYS:HB2	2.06	0.54
1:D:185:ILE:HG23	1:D:345:LYS:CA	2.38	0.54
1:E:113:ILE:HD11	1:E:164:LEU:HD12	1.90	0.54
1:F:157:LEU:O	1:F:163:GLY:HA3	2.07	0.54
1:F:157:LEU:HD12	1:F:163:GLY:N	2.22	0.54
1:A:113:ILE:N	1:A:113:ILE:HD13	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:PHE:CD1	1:C:97:PHE:N	2.74	0.54
1:G:223:LYS:HB2	1:G:223:LYS:NZ	2.23	0.54
1:C:128:ILE:HG13	1:C:128:ILE:O	2.07	0.54
1:C:196:VAL:O	1:C:198:LYS:N	2.41	0.54
1:D:274:LEU:HD13	1:D:274:LEU:O	2.07	0.54
1:F:192:ASP:HB3	1:F:195:GLU:HB2	1.89	0.54
1:B:119:SER:N	1:B:349:ASP:OD1	2.40	0.54
1:C:274:LEU:HD13	1:C:274:LEU:O	2.08	0.54
1:C:330:ALA:N	1:C:331:PRO:CD	2.70	0.54
1:E:225:LEU:HD12	1:E:225:LEU:H	1.72	0.54
1:G:196:VAL:O	1:G:198:LYS:N	2.40	0.54
1:A:225:LEU:N	1:A:225:LEU:HD12	2.23	0.54
1:D:142:SER:O	1:D:315:LEU:HD13	2.08	0.54
1:D:212:MSE:HE1	1:D:260:LYS:HE2	1.90	0.54
1:A:146:GLN:HA	1:A:146:GLN:NE2	2.23	0.53
1:A:146:GLN:HG3	1:A:342:ILE:HD12	1.90	0.53
1:A:215:VAL:HG11	1:A:267:ASP:HB3	1.89	0.53
1:C:286:GLN:HA	1:C:286:GLN:NE2	2.23	0.53
1:B:117:SER:OG	1:B:349:ASP:HA	2.08	0.53
1:B:184:GLU:O	1:B:187:GLN:HG2	2.09	0.53
1:C:230:ARG:HG2	1:C:230:ARG:HH11	1.72	0.53
1:G:327:LEU:H	1:G:327:LEU:CD1	2.21	0.53
1:C:328:ILE:HG22	1:C:328:ILE:O	2.07	0.53
1:D:235:LEU:C	1:D:235:LEU:HD23	2.29	0.53
1:E:170:TRP:HB3	1:E:202:VAL:HG12	1.89	0.53
1:F:214:LEU:HD12	1:F:217:GLN:OE1	2.08	0.53
1:B:99:ARG:NH2	1:C:198:LYS:HG2	2.23	0.53
1:B:212:MSE:HE1	1:B:260:LYS:CD	2.36	0.53
1:C:142:SER:O	1:C:315:LEU:HD13	2.09	0.53
1:D:113:ILE:CD1	1:D:164:LEU:HD12	2.38	0.53
1:G:137:PHE:CZ	1:G:314:TYR:HB2	2.43	0.53
1:A:99:ARG:HH22	4:B:367:GOL:H12	1.73	0.53
1:B:252:GLY:N	3:B:359:IMD:N3	2.56	0.53
1:C:101:ASP:OD1	1:C:102:GLU:N	2.41	0.53
1:D:323:ARG:H	1:D:323:ARG:HD2	1.73	0.53
1:A:146:GLN:HE22	1:A:181:ARG:HE	1.56	0.53
1:B:137:PHE:CZ	1:B:314:TYR:HB2	2.42	0.53
1:D:167:SER:OG	1:D:225:LEU:HD23	2.08	0.53
1:F:265:LEU:HD21	1:F:306:ALA:HA	1.90	0.53
1:A:249:ILE:N	1:A:249:ILE:CD1	2.63	0.53
1:D:154:MSE:SE	1:D:189:ARG:NH1	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:TRP:HB3	1:D:202:VAL:HG12	1.91	0.53
1:G:146:GLN:HG3	1:G:342:ILE:HD12	1.90	0.53
1:G:255:ALA:O	1:G:259:GLN:HG2	2.08	0.53
1:A:42:GLY:CA	1:A:84:ILE:HD11	2.38	0.53
1:G:257:ARG:NH1	1:G:304:ILE:HD13	2.24	0.53
1:C:103:TYR:CE1	1:C:107:ARG:HD2	2.44	0.53
1:B:157:LEU:HD13	1:B:161:GLU:HB3	1.90	0.53
1:D:107:ARG:HD3	1:E:180:GLU:OE2	2.09	0.53
1:D:182:ILE:HB	1:D:197:LEU:HD21	1.91	0.53
1:E:142:SER:O	1:E:315:LEU:HD13	2.09	0.53
1:E:181:ARG:NH1	1:E:346:GLY:HA2	2.23	0.53
1:F:146:GLN:HG3	1:F:342:ILE:HD12	1.91	0.53
1:G:160:GLU:CD	1:G:160:GLU:H	2.12	0.53
1:B:237:VAL:HB	1:B:281:VAL:HG12	1.92	0.52
1:B:320:GLY:HA2	3:B:360:IMD:HN3	1.74	0.52
1:D:183:ARG:O	1:D:185:ILE:N	2.42	0.52
1:A:82:LEU:O	1:A:86:GLN:HG3	2.09	0.52
1:A:170:TRP:HB3	1:A:202:VAL:CG1	2.39	0.52
1:A:251:ARG:HG2	1:B:251:ARG:HG2	1.92	0.52
1:A:324:ILE:HD13	1:A:337:GLU:HB3	1.89	0.52
1:C:187:GLN:HA	1:C:191:LEU:O	2.10	0.52
1:D:222:ILE:N	1:D:222:ILE:CD1	2.72	0.52
1:D:225:LEU:HD12	1:D:225:LEU:H	1.74	0.52
1:E:123:LEU:HG	1:E:327:LEU:HD13	1.91	0.52
1:G:245:ARG:HH22	1:G:283:ASN:HD21	1.58	0.52
1:D:305:LEU:HD23	1:D:305:LEU:O	2.09	0.52
1:D:316:ARG:NH1	1:D:337:GLU:OE2	2.39	0.52
1:A:158:PRO:HD2	1:A:161:GLU:HG3	1.91	0.52
1:B:99:ARG:NE	1:C:198:LYS:HA	2.23	0.52
1:B:112:ARG:HD3	1:B:126:GLY:HA3	1.92	0.52
1:D:192:ASP:OD2	1:D:195:GLU:HB2	2.09	0.52
1:A:179:PRO:HG2	1:G:104:LEU:HD13	1.92	0.52
1:A:222:ILE:HD13	1:A:277:ILE:CD1	2.40	0.52
1:B:252:GLY:N	3:B:359:IMD:HN3	2.07	0.52
1:C:214:LEU:HA	1:C:217:GLN:OE1	2.10	0.52
1:D:344:GLU:O	1:D:345:LYS:CB	2.58	0.52
1:A:184:GLU:O	1:A:186:ALA:N	2.43	0.52
1:B:329:ASP:O	1:B:330:ALA:HB2	2.10	0.52
1:B:332:HIS:HB3	1:B:333:LEU:CD1	2.39	0.52
1:C:184:GLU:HG2	6:C:384:HOH:O	2.10	0.52
1:C:225:LEU:O	1:C:231:PRO:HA	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:LEU:HB2	1:G:179:PRO:CG	2.40	0.52
1:D:326:ARG:NH2	1:D:326:ARG:CB	2.72	0.52
1:G:318:GLY:N	1:G:322:LYS:O	2.31	0.52
1:A:254:LEU:HD13	1:B:249:ILE:HG12	1.92	0.52
1:B:101:ASP:CG	1:B:102:GLU:N	2.63	0.52
1:C:137:PHE:CZ	1:C:314:TYR:HB2	2.45	0.52
1:C:304:ILE:CG1	1:C:305:LEU:N	2.73	0.52
1:A:165:ASN:HA	1:A:230:ARG:HH12	1.75	0.51
1:B:322:LYS:C	1:B:323:ARG:HD2	2.31	0.51
1:E:105:LYS:O	1:E:108:ALA:HB3	2.09	0.51
1:E:207:ASN:HB2	1:E:247:GLU:OE1	2.10	0.51
1:E:230:ARG:HB3	1:E:230:ARG:HH11	1.75	0.51
1:F:316:ARG:HG2	1:F:324:ILE:HG22	1.92	0.51
1:A:331:PRO:CD	1:B:140:PHE:HZ	2.23	0.51
1:C:211:GLN:HE21	1:C:264:HIS:CE1	2.28	0.51
1:E:170:TRP:HB3	1:E:202:VAL:CG1	2.40	0.51
1:F:344:GLU:O	1:F:345:LYS:CB	2.58	0.51
1:A:249:ILE:CD1	1:G:258:GLN:HG3	2.40	0.51
1:B:183:ARG:CG	1:B:193:PRO:HB2	2.40	0.51
1:C:211:GLN:HE21	1:C:264:HIS:HE1	1.57	0.51
1:E:235:LEU:HD23	1:E:235:LEU:C	2.31	0.51
1:F:332:HIS:O	1:F:333:LEU:HB2	2.10	0.51
1:G:207:ASN:HB2	1:G:247:GLU:OE1	2.10	0.51
1:B:254:LEU:H	3:B:359:IMD:H4	1.75	0.51
1:C:323:ARG:HE	1:C:342:ILE:HG13	1.75	0.51
1:G:195:GLU:O	1:G:198:LYS:HB2	2.11	0.51
1:A:317:LYS:HE2	1:A:323:ARG:NH2	2.26	0.51
1:A:344:GLU:O	1:A:345:LYS:CB	2.58	0.51
1:B:99:ARG:HH21	1:C:198:LYS:HG2	1.75	0.51
1:B:320:GLY:HA2	3:B:360:IMD:N3	2.25	0.51
1:F:218:ALA:O	1:F:220:ASP:N	2.43	0.51
1:G:185:ILE:HG13	1:G:345:LYS:C	2.31	0.51
1:D:114:SER:CA	1:D:121:ASP:OD2	2.58	0.51
1:G:117:SER:HB2	1:G:349:ASP:OXT	2.11	0.51
1:G:133:ILE:HD13	1:G:269:HIS:ND1	2.26	0.51
1:D:171:ILE:HD12	1:D:214:LEU:HB3	1.92	0.51
1:D:177:PHE:HE1	1:D:182:ILE:HD11	1.73	0.51
1:G:124:LEU:O	1:G:333:LEU:HD21	2.10	0.51
1:B:182:ILE:HG22	1:B:183:ARG:N	2.26	0.51
1:D:99:ARG:NE	1:D:101:ASP:OD2	2.41	0.51
1:D:128:ILE:HG13	1:D:128:ILE:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:LYS:N	1:E:349:ASP:OD2	2.44	0.51
1:F:221:LYS:HZ2	3:F:363:IMD:H4	1.75	0.51
1:G:316:ARG:NH1	1:G:337:GLU:OE2	2.42	0.51
1:A:169:ILE:HD11	1:A:221:LYS:HG2	1.93	0.51
1:A:241:THR:OG1	1:A:283:ASN:ND2	2.44	0.51
1:B:146:GLN:HG3	1:B:342:ILE:HD12	1.92	0.51
1:B:178:ARG:HB2	1:B:181:ARG:HB3	1.93	0.51
1:B:251:ARG:O	1:B:253:ALA:N	2.44	0.51
1:F:258:GLN:HE21	1:F:258:GLN:CA	2.00	0.51
1:B:142:SER:O	1:B:315:LEU:HD13	2.11	0.51
1:F:179:PRO:HG2	1:F:180:GLU:OE2	2.11	0.50
1:F:237:VAL:HB	1:F:281:VAL:HG12	1.92	0.50
1:G:142:SER:O	1:G:315:LEU:HD13	2.11	0.50
1:E:316:ARG:NH1	1:E:324:ILE:HD12	2.27	0.50
1:F:184:GLU:OE2	1:F:344:GLU:HA	2.11	0.50
1:G:187:GLN:O	1:G:187:GLN:HG3	2.12	0.50
1:A:37:ILE:HG12	1:A:38:GLU:N	2.26	0.50
1:A:212:MSE:HE1	1:A:260:LYS:CD	2.36	0.50
1:A:331:PRO:HD3	1:B:140:PHE:CZ	2.46	0.50
1:B:177:PHE:CE1	1:B:182:ILE:HD12	2.46	0.50
1:C:187:GLN:HB3	1:C:193:PRO:CD	2.40	0.50
1:D:207:ASN:HA	1:D:243:HIS:ND1	2.27	0.50
1:E:120:LEU:HD22	1:E:124:LEU:CD1	2.41	0.50
1:G:215:VAL:HG21	1:G:264:HIS:NE2	2.26	0.50
1:B:101:ASP:OD1	1:B:102:GLU:N	2.44	0.50
1:B:274:LEU:HD12	1:B:275:TYR:CE2	2.47	0.50
1:F:322:LYS:O	1:F:323:ARG:NH1	2.44	0.50
1:A:304:ILE:HG13	1:A:305:LEU:N	2.27	0.50
1:C:258:GLN:O	1:C:259:GLN:C	2.49	0.50
1:D:252:GLY:HA2	6:D:385:HOH:O	2.11	0.50
1:D:327:LEU:CD1	1:D:333:LEU:HB3	2.42	0.50
1:A:142:SER:O	1:A:315:LEU:HD13	2.11	0.50
1:A:228:THR:HG22	1:A:230:ARG:H	1.76	0.50
1:A:286:GLN:HG3	1:A:286:GLN:O	2.12	0.50
1:D:137:PHE:CZ	1:D:314:TYR:HB2	2.46	0.50
1:F:100:ALA:HB3	1:G:197:LEU:HA	1.94	0.50
1:F:101:ASP:OD2	1:F:102:GLU:HG2	2.10	0.50
1:B:330:ALA:N	1:B:331:PRO:HD2	2.15	0.50
1:F:330:ALA:H	1:F:331:PRO:HD2	1.75	0.50
1:G:187:GLN:HB3	1:G:193:PRO:HG3	1.92	0.50
1:B:248:TYR:OH	1:B:260:LYS:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLU:O	1:B:345:LYS:CB	2.60	0.50
1:C:146:GLN:HG3	1:C:342:ILE:HD12	1.93	0.50
1:G:178:ARG:O	1:G:181:ARG:HB3	2.11	0.50
1:D:112:ARG:HD2	1:D:126:GLY:HA3	1.93	0.50
1:A:37:ILE:HG23	1:A:39:ASP:OD2	2.12	0.49
1:B:158:PRO:O	1:B:161:GLU:HB2	2.12	0.49
1:C:269:HIS:HB3	1:D:206:PHE:CD2	2.47	0.49
1:E:99:ARG:HE	1:F:198:LYS:HA	1.77	0.49
1:E:156:GLN:OE1	1:E:199:HIS:HB2	2.12	0.49
1:E:274:LEU:HD12	1:E:275:TYR:CE2	2.47	0.49
1:A:107:ARG:HH21	1:B:178:ARG:CZ	2.25	0.49
1:A:215:VAL:O	1:A:218:ALA:HB3	2.11	0.49
1:D:326:ARG:HG2	1:D:327:LEU:H	1.76	0.49
1:F:169:ILE:HD11	1:F:221:LYS:HG2	1.94	0.49
1:C:230:ARG:HG2	1:C:230:ARG:NH1	2.27	0.49
1:F:219:GLU:CD	1:F:270:ARG:HH22	2.14	0.49
1:A:257:ARG:NH2	1:A:304:ILE:HD13	2.27	0.49
1:A:264:HIS:HD2	6:A:429:HOH:O	1.94	0.49
1:B:146:GLN:HE21	1:B:146:GLN:CA	2.20	0.49
1:B:254:LEU:HD21	1:C:249:ILE:HG21	1.94	0.49
1:C:324:ILE:HD11	1:C:337:GLU:HB3	1.93	0.49
1:E:192:ASP:HB3	1:E:195:GLU:HB2	1.94	0.49
1:F:201:TYR:CD1	1:F:201:TYR:N	2.81	0.49
1:F:304:ILE:HG22	1:F:305:LEU:N	2.27	0.49
1:F:324:ILE:HD13	1:F:324:ILE:C	2.33	0.49
1:G:330:ALA:HB3	1:G:331:PRO:CD	2.41	0.49
1:G:348:GLU:O	1:G:349:ASP:CB	2.57	0.49
1:D:223:LYS:HB2	1:D:223:LYS:HZ2	1.77	0.49
1:F:166:GLY:HA3	1:F:233:LYS:HG3	1.95	0.49
1:F:318:GLY:O	1:F:319:LYS:C	2.51	0.49
1:G:179:PRO:O	1:G:182:ILE:HB	2.13	0.49
1:G:184:GLU:HG2	1:G:185:ILE:N	2.27	0.49
1:C:181:ARG:HH21	1:C:181:ARG:HG3	1.76	0.49
1:D:142:SER:O	1:D:323:ARG:HG2	2.12	0.49
1:E:145:THR:HG23	1:E:238:ASP:OD2	2.13	0.49
1:A:118:LYS:N	1:A:349:ASP:OXT	2.46	0.49
1:C:330:ALA:H	1:C:331:PRO:CD	2.17	0.49
1:E:120:LEU:HD22	1:E:124:LEU:HD11	1.94	0.49
1:E:254:LEU:HD12	1:E:254:LEU:O	2.13	0.49
1:F:157:LEU:HD12	1:F:163:GLY:H	1.77	0.49
1:F:185:ILE:HG23	1:F:345:LYS:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:HD3	1:A:337:GLU:CG	2.37	0.49
1:C:185:ILE:HD13	6:C:384:HOH:O	2.12	0.49
1:G:201:TYR:N	1:G:201:TYR:CD1	2.80	0.49
1:A:348:GLU:O	1:A:349:ASP:HB2	2.12	0.49
1:E:118:LYS:HB2	1:E:349:ASP:OD2	2.12	0.49
1:E:133:ILE:HD13	1:E:269:HIS:ND1	2.28	0.49
1:B:249:ILE:HD13	1:B:249:ILE:H	1.78	0.49
1:B:316:ARG:NH1	1:B:326:ARG:NH2	2.61	0.49
1:B:328:ILE:N	1:B:328:ILE:CD1	2.70	0.49
1:C:188:ASN:OD1	1:C:344:GLU:CB	2.61	0.49
1:C:250:GLY:O	1:C:253:ALA:HB3	2.12	0.49
1:D:214:LEU:O	1:D:218:ALA:HB2	2.13	0.49
1:F:144:LYS:HG2	2:F:355:SO4:O4	2.12	0.49
1:D:245:ARG:NH1	1:D:304:ILE:HG22	2.28	0.48
1:F:99:ARG:HD2	1:G:198:LYS:O	2.12	0.48
1:F:250:GLY:O	1:F:253:ALA:HB3	2.12	0.48
1:D:101:ASP:OD1	1:D:102:GLU:N	2.45	0.48
1:F:147:LEU:HA	1:F:347:ILE:CD1	2.43	0.48
1:F:221:LYS:HZ3	3:F:363:IMD:H4	1.75	0.48
1:F:333:LEU:HB3	1:F:334:PRO:HD2	1.96	0.48
1:G:160:GLU:N	1:G:160:GLU:OE1	2.46	0.48
1:G:332:HIS:O	1:G:333:LEU:CB	2.53	0.48
1:A:52:ARG:C	1:A:54:ALA:H	2.16	0.48
1:A:241:THR:HB	1:A:304:ILE:HG21	1.95	0.48
1:B:123:LEU:CD1	1:B:334:PRO:HG2	2.42	0.48
1:B:189:ARG:HG3	1:B:345:LYS:HG2	1.96	0.48
1:B:326:ARG:HG2	1:B:327:LEU:N	2.28	0.48
1:E:324:ILE:HD13	1:E:324:ILE:C	2.34	0.48
1:B:205:ALA:O	1:B:243:HIS:HE1	1.97	0.48
1:B:314:TYR:HB3	1:B:328:ILE:HD11	1.93	0.48
1:D:182:ILE:HD13	1:D:200:ILE:CD1	2.41	0.48
1:C:117:SER:HB2	1:C:349:ASP:OD2	2.13	0.48
1:C:147:LEU:HD22	1:C:151:LEU:HD22	1.96	0.48
1:C:166:GLY:HA3	1:C:233:LYS:HG3	1.96	0.48
1:C:225:LEU:H	1:C:225:LEU:CD2	2.25	0.48
1:E:102:GLU:O	1:E:105:LYS:HB3	2.13	0.48
1:A:180:GLU:HG3	1:G:104:LEU:CD1	2.44	0.48
1:B:245:ARG:NH1	1:B:304:ILE:HG22	2.29	0.48
1:C:111:GLY:CA	6:C:404:HOH:O	2.60	0.48
1:C:344:GLU:O	1:C:345:LYS:CB	2.61	0.48
1:D:313:VAL:HG22	1:D:327:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:TYR:HB3	1:E:328:ILE:HD11	1.96	0.48
1:E:331:PRO:HG3	1:F:140:PHE:CZ	2.48	0.48
1:B:225:LEU:O	1:B:228:THR:HB	2.14	0.48
1:D:182:ILE:HD12	1:D:197:LEU:CD2	2.44	0.48
1:E:212:MSE:HE1	1:E:260:LYS:HD3	1.94	0.48
1:F:117:SER:HB2	1:F:348:GLU:O	2.13	0.48
1:F:207:ASN:HA	1:F:243:HIS:ND1	2.28	0.48
1:F:258:GLN:NE2	1:F:258:GLN:CA	2.64	0.48
1:G:105:LYS:O	1:G:108:ALA:HB3	2.14	0.48
1:G:188:ASN:O	1:G:345:LYS:HG2	2.14	0.48
1:A:98:MSE:HG2	1:A:102:GLU:HB3	1.96	0.48
1:B:101:ASP:HB3	1:C:197:LEU:O	2.14	0.48
1:D:157:LEU:O	1:D:163:GLY:HA3	2.13	0.48
1:F:189:ARG:HG3	1:F:189:ARG:NH2	2.29	0.48
1:F:226:LEU:C	1:F:226:LEU:HD13	2.34	0.48
1:G:108:ALA:C	1:G:110:ILE:H	2.17	0.48
1:G:192:ASP:OD2	1:G:195:GLU:HB2	2.14	0.48
1:B:201:TYR:CD1	1:B:201:TYR:N	2.81	0.48
1:C:144:LYS:HG2	2:C:352:SO4:O4	2.14	0.48
1:C:195:GLU:HA	1:C:198:LYS:HD2	1.95	0.48
1:G:146:GLN:HE22	1:G:181:ARG:HE	1.62	0.48
1:C:235:LEU:HD23	1:C:235:LEU:C	2.34	0.47
1:D:201:TYR:CD1	1:D:201:TYR:N	2.82	0.47
1:E:243:HIS:O	1:E:247:GLU:HG3	2.13	0.47
1:G:121:ASP:HB3	1:G:126:GLY:O	2.14	0.47
1:G:331:PRO:O	1:G:332:HIS:HB2	2.13	0.47
1:A:117:SER:O	1:A:121:ASP:OD1	2.32	0.47
1:A:304:ILE:HG13	1:A:305:LEU:H	1.79	0.47
1:C:241:THR:OG1	1:C:283:ASN:ND2	2.47	0.47
1:C:316:ARG:NH1	1:C:337:GLU:OE2	2.43	0.47
1:G:211:GLN:HE21	1:G:264:HIS:HE1	1.62	0.47
1:B:333:LEU:HD12	1:B:333:LEU:N	2.29	0.47
1:D:211:GLN:HE21	1:D:264:HIS:CE1	2.33	0.47
1:D:241:THR:OG1	1:D:283:ASN:ND2	2.47	0.47
1:E:238:ASP:HA	1:E:239:SER:HA	1.74	0.47
1:F:147:LEU:HA	1:F:347:ILE:HD11	1.97	0.47
1:G:225:LEU:HD12	1:G:228:THR:HB	1.96	0.47
1:D:133:ILE:HD13	1:D:269:HIS:ND1	2.29	0.47
1:F:188:ASN:ND2	1:F:344:GLU:HG2	2.29	0.47
1:G:316:ARG:NH1	1:G:326:ARG:HH21	2.13	0.47
1:A:197:LEU:HD11	1:G:104:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ALA:HB1	1:C:193:PRO:HA	1.96	0.47
1:F:274:LEU:HD12	1:F:275:TYR:CE2	2.49	0.47
1:A:243:HIS:O	1:A:247:GLU:HG3	2.14	0.47
1:A:274:LEU:HD12	1:A:275:TYR:CE2	2.49	0.47
1:C:111:GLY:N	6:C:404:HOH:O	2.47	0.47
1:E:201:TYR:CD1	1:E:201:TYR:N	2.82	0.47
1:F:113:ILE:HD11	1:F:164:LEU:CD1	2.43	0.47
1:F:211:GLN:HE21	1:F:264:HIS:CE1	2.33	0.47
1:G:164:LEU:O	1:G:165:ASN:C	2.52	0.47
1:A:76:ILE:HD13	1:A:76:ILE:N	2.30	0.47
1:A:115:THR:CB	1:A:120:LEU:HD23	2.44	0.47
1:A:201:TYR:N	1:A:201:TYR:CD1	2.83	0.47
1:A:225:LEU:O	1:A:228:THR:HB	2.15	0.47
1:B:183:ARG:HG2	1:B:183:ARG:HH11	1.80	0.47
1:B:188:ASN:OD1	1:B:344:GLU:HB3	2.14	0.47
1:B:302:GLY:C	1:B:304:ILE:N	2.67	0.47
1:D:189:ARG:NE	1:D:345:LYS:HB3	2.28	0.47
1:E:123:LEU:HG	1:E:327:LEU:CD1	2.45	0.47
1:F:211:GLN:HE21	1:F:264:HIS:HE1	1.62	0.47
1:G:157:LEU:O	1:G:163:GLY:HA3	2.14	0.47
1:G:241:THR:OG1	1:G:283:ASN:ND2	2.48	0.47
1:G:251:ARG:HD3	1:G:252:GLY:N	2.29	0.47
1:A:251:ARG:HG3	1:A:251:ARG:NH1	2.29	0.47
1:B:304:ILE:HD13	1:B:304:ILE:C	2.34	0.47
1:G:228:THR:CG2	1:G:229:ASP:N	2.78	0.47
1:A:228:THR:CG2	1:A:229:ASP:N	2.77	0.47
1:C:254:LEU:HD12	1:C:254:LEU:O	2.14	0.47
1:D:348:GLU:O	1:D:349:ASP:HB2	2.14	0.47
1:E:333:LEU:HD12	1:E:334:PRO:HD2	1.97	0.47
1:F:235:LEU:C	1:F:235:LEU:HD23	2.35	0.47
1:F:241:THR:OG1	1:F:283:ASN:ND2	2.47	0.47
1:A:230:ARG:NH1	1:A:230:ARG:HG2	2.30	0.47
1:A:249:ILE:HD12	1:A:249:ILE:H	1.73	0.47
1:D:183:ARG:C	1:D:185:ILE:N	2.68	0.47
1:C:123:LEU:HD21	1:C:336:GLY:O	2.14	0.46
1:C:328:ILE:O	1:C:329:ASP:HB3	2.15	0.46
1:E:213:LEU:O	1:E:217:GLN:HG3	2.14	0.46
1:E:327:LEU:O	1:E:328:ILE:HD12	2.15	0.46
1:F:332:HIS:C	1:F:333:LEU:HD12	2.35	0.46
1:A:137:PHE:CZ	1:A:314:TYR:HB2	2.49	0.46
1:D:170:TRP:CE3	1:D:236:ILE:HD12	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ILE:HG12	1:D:305:LEU:N	2.30	0.46
1:F:243:HIS:O	1:F:247:GLU:HG3	2.14	0.46
1:C:192:ASP:OD2	1:C:195:GLU:HB2	2.15	0.46
1:D:97:PHE:HE2	1:E:171:ILE:CD1	2.27	0.46
1:D:146:GLN:HE22	1:D:181:ARG:HE	1.63	0.46
1:E:331:PRO:CG	1:F:140:PHE:HZ	2.29	0.46
1:F:104:LEU:HB2	1:G:179:PRO:HB2	1.96	0.46
1:F:171:ILE:HD12	1:F:214:LEU:HB3	1.97	0.46
1:F:180:GLU:H	1:F:180:GLU:CD	2.18	0.46
1:F:219:GLU:O	1:F:223:LYS:HG3	2.15	0.46
1:G:235:LEU:C	1:G:235:LEU:HD23	2.36	0.46
1:C:187:GLN:CB	1:C:193:PRO:HD3	2.44	0.46
1:C:201:TYR:CD1	1:C:201:TYR:N	2.83	0.46
1:A:104:LEU:HD12	1:B:180:GLU:HG3	1.98	0.46
1:F:156:GLN:OE1	1:F:199:HIS:HB2	2.15	0.46
1:G:192:ASP:HA	1:G:193:PRO:HD2	1.74	0.46
1:C:348:GLU:HG2	1:C:349:ASP:N	2.30	0.46
1:D:332:HIS:CE1	1:E:178:ARG:NE	2.78	0.46
1:A:124:LEU:HD12	1:A:127:GLY:HA2	1.97	0.46
1:B:99:ARG:NE	1:B:101:ASP:OD2	2.48	0.46
1:B:166:GLY:HA3	1:B:233:LYS:HG3	1.98	0.46
1:C:274:LEU:HD12	1:C:275:TYR:CE2	2.51	0.46
1:G:327:LEU:N	1:G:327:LEU:CD1	2.79	0.46
1:G:329:ASP:HB3	1:G:330:ALA:H	1.52	0.46
1:A:158:PRO:HB3	1:A:160:GLU:OE1	2.16	0.46
1:B:235:LEU:C	1:B:235:LEU:HD23	2.36	0.46
1:E:332:HIS:O	1:E:333:LEU:CB	2.63	0.46
1:A:80:THR:O	1:A:84:ILE:HG12	2.15	0.46
1:B:187:GLN:HG3	1:B:188:ASN:H	1.79	0.46
1:C:225:LEU:C	1:C:231:PRO:HA	2.35	0.46
1:C:316:ARG:HG2	1:C:324:ILE:HG23	1.98	0.46
1:D:187:GLN:NE2	1:D:193:PRO:HG3	2.31	0.46
1:D:313:VAL:HG22	1:D:327:LEU:CD2	2.46	0.46
1:D:323:ARG:HD2	1:D:323:ARG:N	2.31	0.46
1:E:237:VAL:HB	1:E:281:VAL:HG12	1.98	0.46
1:G:120:LEU:CD2	1:G:124:LEU:HD12	2.45	0.46
1:A:189:ARG:NH2	1:A:345:LYS:O	2.49	0.46
1:B:189:ARG:NE	1:B:345:LYS:HB3	2.30	0.46
1:C:119:SER:O	1:C:122:LYS:HB3	2.15	0.46
1:D:186:ALA:O	1:D:188:ASN:N	2.40	0.46
1:E:286:GLN:H	1:E:303:HIS:HE1	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:PHE:HB2	1:G:284:GLN:OE1	2.16	0.46
1:B:137:PHE:HZ	1:B:328:ILE:HG12	1.82	0.45
1:D:207:ASN:CA	1:D:243:HIS:ND1	2.79	0.45
1:D:221:LYS:O	1:D:225:LEU:HD13	2.16	0.45
1:F:118:LYS:O	1:F:122:LYS:HG3	2.16	0.45
1:A:221:LYS:HG3	1:A:225:LEU:CD1	2.41	0.45
1:B:323:ARG:HE	1:B:342:ILE:CG1	2.26	0.45
1:E:133:ILE:HD11	1:E:269:HIS:HA	1.99	0.45
1:E:211:GLN:HE21	1:E:264:HIS:CE1	2.33	0.45
1:E:230:ARG:HH11	1:E:230:ARG:CB	2.28	0.45
1:A:146:GLN:HE22	1:A:181:ARG:NE	2.14	0.45
1:B:285:VAL:HG13	1:B:285:VAL:O	2.16	0.45
1:D:326:ARG:NH1	1:D:337:GLU:OE2	2.49	0.45
1:G:243:HIS:O	1:G:247:GLU:HG3	2.16	0.45
1:C:237:VAL:HB	1:C:281:VAL:HG12	1.98	0.45
1:C:322:LYS:HG2	1:C:341:SER:HB3	1.98	0.45
1:D:243:HIS:O	1:D:247:GLU:HG3	2.16	0.45
1:F:157:LEU:HD13	1:F:161:GLU:HB3	1.98	0.45
1:G:106:LYS:C	1:G:108:ALA:H	2.20	0.45
1:G:303:HIS:CG	1:G:304:ILE:N	2.84	0.45
1:A:77:SER:OG	1:A:80:THR:HG23	2.17	0.45
1:A:99:ARG:O	1:A:102:GLU:N	2.49	0.45
1:A:158:PRO:HA	1:A:159:PRO:HD3	1.86	0.45
1:C:158:PRO:HA	1:C:159:PRO:HD3	1.85	0.45
1:E:158:PRO:HD2	1:E:161:GLU:HG3	1.98	0.45
1:A:156:GLN:OE1	1:A:199:HIS:HB2	2.16	0.45
1:A:160:GLU:OE2	1:A:160:GLU:N	2.49	0.45
1:A:258:GLN:CG	1:B:249:ILE:HD11	2.47	0.45
1:C:269:HIS:HB3	1:D:206:PHE:CE2	2.52	0.45
1:G:305:LEU:HG	1:G:306:ALA:N	2.31	0.45
1:A:43:VAL:HG23	1:A:84:ILE:HD12	1.98	0.45
1:B:182:ILE:HD13	1:B:200:ILE:CD1	2.47	0.45
1:B:185:ILE:HA	6:B:386:HOH:O	2.16	0.45
1:D:307:HIS:ND1	1:D:308:SER:N	2.65	0.45
1:E:211:GLN:HE21	1:E:264:HIS:HE1	1.64	0.45
1:F:245:ARG:HB3	1:F:304:ILE:CD1	2.41	0.45
1:G:344:GLU:O	1:G:345:LYS:CB	2.61	0.45
1:B:182:ILE:O	1:B:183:ARG:C	2.54	0.45
1:C:159:PRO:HA	1:C:163:GLY:O	2.17	0.45
1:D:169:ILE:HG13	1:D:222:ILE:CD1	2.33	0.45
1:D:185:ILE:O	1:D:189:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:LEU:CD1	1:E:334:PRO:HD2	2.47	0.45
1:G:274:LEU:HD12	1:G:275:TYR:CE2	2.52	0.45
1:A:251:ARG:HE	1:B:251:ARG:HH22	1.64	0.45
1:A:265:LEU:HD21	1:A:306:ALA:HA	1.98	0.45
1:D:211:GLN:HE21	1:D:264:HIS:HE1	1.65	0.45
1:D:305:LEU:HB2	1:D:312:ARG:HH21	1.82	0.45
1:E:117:SER:HB3	1:E:347:ILE:HG22	1.98	0.45
1:F:170:TRP:CE3	1:F:236:ILE:HD12	2.52	0.45
1:A:146:GLN:HG2	6:A:421:HOH:O	2.17	0.45
1:A:164:LEU:O	1:A:165:ASN:C	2.56	0.45
1:A:318:GLY:O	1:A:319:LYS:C	2.54	0.45
1:A:324:ILE:HD12	1:A:325:ALA:N	2.32	0.45
1:B:115:THR:HA	1:B:151:LEU:CD1	2.47	0.45
1:B:219:GLU:CD	1:B:270:ARG:NH2	2.69	0.45
1:D:158:PRO:HA	1:D:159:PRO:HD3	1.81	0.45
1:A:49:GLU:OE2	1:A:49:GLU:HA	2.15	0.44
1:A:258:GLN:HG3	1:B:249:ILE:HD11	1.99	0.44
1:C:181:ARG:CZ	1:C:185:ILE:HD11	2.47	0.44
1:F:142:SER:O	1:F:315:LEU:HD13	2.17	0.44
1:F:218:ALA:O	1:F:221:LYS:N	2.50	0.44
1:B:97:PHE:O	1:B:98:MSE:C	2.56	0.44
1:C:224:GLU:N	1:C:224:GLU:OE1	2.50	0.44
1:D:166:GLY:HA3	1:D:233:LYS:HG3	1.99	0.44
1:D:328:ILE:O	1:D:329:ASP:HB3	2.16	0.44
1:F:140:PHE:HB2	1:F:284:GLN:OE1	2.17	0.44
1:F:146:GLN:NE2	1:F:181:ARG:HE	2.15	0.44
1:F:222:ILE:N	1:F:222:ILE:HD12	2.32	0.44
1:G:238:ASP:HA	1:G:239:SER:HA	1.70	0.44
1:B:179:PRO:HD2	1:B:180:GLU:OE1	2.16	0.44
1:D:115:THR:O	1:D:150:THR:HG21	2.17	0.44
1:E:101:ASP:OD1	1:E:102:GLU:N	2.50	0.44
1:F:192:ASP:O	1:F:195:GLU:N	2.49	0.44
1:A:113:ILE:HD12	1:A:164:LEU:HG	1.98	0.44
1:A:286:GLN:NE2	1:A:286:GLN:CA	2.80	0.44
1:B:123:LEU:HA	1:B:334:PRO:HG3	1.98	0.44
1:B:183:ARG:HG2	1:B:183:ARG:NH1	2.33	0.44
1:C:181:ARG:NH2	1:C:181:ARG:HG3	2.32	0.44
1:E:250:GLY:O	1:E:253:ALA:HB3	2.16	0.44
1:F:207:ASN:CA	1:F:243:HIS:ND1	2.81	0.44
1:G:285:VAL:O	1:G:285:VAL:HG13	2.18	0.44
1:A:243:HIS:HD2	1:G:307:HIS:HE1	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ILE:O	1:C:329:ASP:CB	2.65	0.44
1:G:192:ASP:O	1:G:194:ASP:N	2.50	0.44
1:B:160:GLU:CD	1:B:160:GLU:H	2.20	0.44
1:B:181:ARG:HD2	1:B:181:ARG:O	2.16	0.44
1:B:210:HIS:O	1:B:213:LEU:HB3	2.18	0.44
1:E:241:THR:OG1	1:E:283:ASN:ND2	2.51	0.44
1:A:107:ARG:HH21	1:B:178:ARG:NE	2.16	0.44
1:A:245:ARG:NH1	1:A:304:ILE:HG22	2.32	0.44
1:B:185:ILE:O	1:B:189:ARG:HB2	2.18	0.44
1:B:254:LEU:H	3:B:359:IMD:C4	2.31	0.44
1:G:99:ARG:CB	1:G:99:ARG:HH11	2.31	0.44
1:A:320:GLY:HA2	3:A:361:IMD:HN3	1.82	0.44
1:A:332:HIS:O	1:A:333:LEU:CB	2.59	0.44
1:D:195:GLU:HA	1:D:198:LYS:HD2	1.99	0.44
1:F:222:ILE:O	1:F:226:LEU:HB2	2.17	0.44
1:B:212:MSE:O	1:B:216:GLN:HG3	2.17	0.44
1:B:251:ARG:HG2	1:B:251:ARG:HH21	1.83	0.44
1:E:113:ILE:O	1:E:127:GLY:HA3	2.18	0.44
1:A:97:PHE:HE2	1:B:171:ILE:CD1	2.31	0.43
1:A:201:TYR:CZ	1:A:225:LEU:HD21	2.53	0.43
1:B:187:GLN:CG	1:B:188:ASN:N	2.80	0.43
1:C:160:GLU:CD	1:C:160:GLU:H	2.20	0.43
1:C:186:ALA:CB	1:C:193:PRO:HA	2.48	0.43
1:C:285:VAL:O	1:C:285:VAL:HG13	2.18	0.43
1:F:123:LEU:HD22	1:F:338:ALA:CB	2.48	0.43
1:A:133:ILE:HD13	1:A:269:HIS:ND1	2.33	0.43
1:B:340:PHE:CD1	1:B:347:ILE:HG23	2.53	0.43
1:D:329:ASP:HB2	1:D:331:PRO:HD2	2.00	0.43
1:G:182:ILE:CG2	1:G:196:VAL:HG11	2.48	0.43
1:G:257:ARG:O	1:G:261:LEU:HB2	2.18	0.43
1:A:251:ARG:HG2	1:B:251:ARG:CG	2.48	0.43
1:B:170:TRP:CE3	1:B:236:ILE:HD12	2.54	0.43
1:C:140:PHE:HB2	1:C:284:GLN:OE1	2.18	0.43
1:C:265:LEU:HD21	1:C:306:ALA:HB1	1.99	0.43
1:E:166:GLY:HA3	1:E:233:LYS:HG3	1.99	0.43
1:E:185:ILE:HG23	1:E:345:LYS:C	2.38	0.43
1:E:331:PRO:HG3	1:F:140:PHE:HZ	1.83	0.43
1:F:286:GLN:CD	1:F:286:GLN:N	2.72	0.43
1:G:327:LEU:C	1:G:328:ILE:HD12	2.37	0.43
1:A:52:ARG:C	1:A:54:ALA:N	2.71	0.43
1:A:147:LEU:HA	1:A:347:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HD12	1:A:233:LYS:HD3	2.00	0.43
1:D:170:TRP:HB3	1:D:202:VAL:HG13	2.00	0.43
1:D:323:ARG:NH1	1:D:323:ARG:HG3	2.34	0.43
1:E:334:PRO:C	1:E:335:GLU:HG3	2.38	0.43
1:F:104:LEU:HB2	1:G:179:PRO:CB	2.48	0.43
1:F:115:THR:HA	1:F:151:LEU:CD1	2.48	0.43
1:A:158:PRO:O	1:A:161:GLU:HB2	2.18	0.43
1:A:201:TYR:CD2	1:A:221:LYS:HD3	2.53	0.43
1:C:251:ARG:CZ	1:D:251:ARG:HA	2.47	0.43
1:D:196:VAL:C	1:D:198:LYS:H	2.21	0.43
1:F:129:GLU:HG3	6:F:396:HOH:O	2.19	0.43
1:C:224:GLU:O	1:C:226:LEU:N	2.51	0.43
1:F:196:VAL:C	1:F:198:LYS:H	2.22	0.43
1:F:240:LEU:HD21	1:F:265:LEU:HD11	2.00	0.43
1:F:269:HIS:NE2	1:F:308:SER:HB3	2.34	0.43
1:G:115:THR:O	1:G:150:THR:HG21	2.19	0.43
1:G:196:VAL:C	1:G:198:LYS:N	2.70	0.43
1:A:323:ARG:HG3	1:A:323:ARG:HH11	1.83	0.43
1:B:118:LYS:N	1:B:349:ASP:HB2	2.27	0.43
1:B:219:GLU:OE1	1:B:270:ARG:NH2	2.52	0.43
1:B:322:LYS:HZ2	1:B:341:SER:HB3	1.82	0.43
1:C:263:LYS:HD3	1:C:267:ASP:OD2	2.17	0.43
1:D:115:THR:HA	1:D:151:LEU:CD1	2.49	0.43
1:D:123:LEU:HD23	1:D:123:LEU:C	2.38	0.43
1:D:193:PRO:HA	1:D:196:VAL:HG23	2.00	0.43
1:E:269:HIS:HB3	1:F:206:PHE:CD2	2.53	0.43
1:A:168:VAL:HG22	1:A:234:LEU:HB3	1.99	0.43
1:A:303:HIS:ND1	1:A:303:HIS:C	2.72	0.43
1:B:147:LEU:HD22	1:B:151:LEU:HD22	2.01	0.43
1:B:238:ASP:HA	1:B:239:SER:HA	1.72	0.43
1:C:101:ASP:O	1:C:104:LEU:HB3	2.18	0.43
1:C:124:LEU:HA	1:C:333:LEU:HD23	2.00	0.43
1:D:97:PHE:HE2	1:E:171:ILE:HD13	1.82	0.43
1:D:328:ILE:HD12	1:D:328:ILE:N	2.33	0.43
1:E:113:ILE:N	1:E:113:ILE:HD13	2.33	0.43
1:G:324:ILE:HD11	1:G:337:GLU:HB3	2.01	0.43
1:D:237:VAL:HB	1:D:281:VAL:HG12	2.01	0.43
1:F:98:MSE:O	1:G:201:TYR:HA	2.19	0.43
1:A:98:MSE:CG	1:A:102:GLU:HB3	2.48	0.43
1:B:128:ILE:O	1:B:128:ILE:HG13	2.17	0.43
1:B:243:HIS:O	1:B:247:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:LEU:HD22	1:D:151:LEU:HD22	2.01	0.43
1:D:340:PHE:HA	1:D:349:ASP:C	2.39	0.43
1:A:171:ILE:CD1	1:G:97:PHE:CE1	3.00	0.42
1:B:316:ARG:HG2	1:B:324:ILE:HG23	2.01	0.42
1:C:265:LEU:HD21	1:C:306:ALA:CB	2.49	0.42
1:E:324:ILE:HA	1:E:338:ALA:O	2.19	0.42
1:F:305:LEU:N	1:F:305:LEU:HD23	2.33	0.42
1:B:187:GLN:C	1:B:189:ARG:N	2.71	0.42
1:B:207:ASN:HB2	1:B:247:GLU:OE1	2.19	0.42
1:C:119:SER:H	1:C:349:ASP:CG	2.21	0.42
1:F:218:ALA:O	1:F:222:ILE:HD13	2.19	0.42
1:B:118:LYS:HB2	1:B:349:ASP:CG	2.39	0.42
1:B:274:LEU:HD13	1:B:274:LEU:O	2.19	0.42
1:D:140:PHE:HB2	1:D:284:GLN:OE1	2.19	0.42
1:D:274:LEU:HD12	1:D:275:TYR:CE2	2.54	0.42
1:F:100:ALA:HB2	1:G:200:ILE:HB	2.00	0.42
1:B:223:LYS:O	1:B:226:LEU:CB	2.67	0.42
1:C:222:ILE:CG2	1:C:277:ILE:HD11	2.49	0.42
1:D:146:GLN:HE21	1:D:146:GLN:CA	2.23	0.42
1:D:324:ILE:HB	1:D:339:VAL:HG22	1.99	0.42
1:G:340:PHE:CD1	1:G:347:ILE:HG23	2.54	0.42
1:A:105:LYS:HE3	1:A:105:LYS:HA	2.02	0.42
1:B:228:THR:CG2	1:B:229:ASP:N	2.82	0.42
1:C:221:LYS:O	1:C:225:LEU:HD23	2.19	0.42
1:C:340:PHE:CD1	1:C:347:ILE:HG23	2.54	0.42
1:B:105:LYS:NZ	1:B:109:THR:HG21	2.34	0.42
1:B:147:LEU:HA	1:B:347:ILE:CD1	2.49	0.42
1:B:223:LYS:O	1:B:226:LEU:HB3	2.20	0.42
1:D:112:ARG:HD3	1:D:125:GLY:O	2.20	0.42
1:F:227:ASN:H	1:F:227:ASN:ND2	2.18	0.42
1:F:251:ARG:N	1:F:251:ARG:CD	2.79	0.42
1:F:320:GLY:C	1:F:322:LYS:H	2.23	0.42
1:A:333:LEU:HB3	1:A:334:PRO:HD2	2.02	0.42
1:B:188:ASN:HD22	1:B:188:ASN:HA	1.59	0.42
1:E:170:TRP:CE3	1:E:236:ILE:HD12	2.55	0.42
1:E:331:PRO:HB3	1:F:140:PHE:HZ	1.85	0.42
1:F:147:LEU:HG	1:F:347:ILE:CD1	2.50	0.42
1:A:97:PHE:CD1	1:A:97:PHE:N	2.88	0.42
1:A:235:LEU:C	1:A:235:LEU:HD23	2.40	0.42
1:C:316:ARG:HG2	1:C:324:ILE:CG2	2.50	0.42
1:D:265:LEU:HA	1:D:265:LEU:HD12	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:SER:OG	1:A:69:GLU:HG3	2.20	0.42
1:A:225:LEU:N	1:A:225:LEU:CD1	2.83	0.42
1:A:323:ARG:NH1	1:A:323:ARG:HG3	2.34	0.42
1:B:186:ALA:HB2	1:B:196:VAL:HG21	2.01	0.42
1:C:219:GLU:CD	1:C:270:ARG:HH22	2.23	0.42
1:E:123:LEU:CG	1:E:327:LEU:HD13	2.50	0.42
1:E:147:LEU:HA	1:E:347:ILE:CD1	2.50	0.42
1:F:190:GLY:C	1:F:191:LEU:HD23	2.40	0.42
1:F:330:ALA:N	1:F:331:PRO:CD	2.82	0.42
1:B:323:ARG:NH2	1:B:323:ARG:HG3	2.32	0.42
1:D:139:GLU:CD	1:D:286:GLN:HG2	2.38	0.42
1:E:115:THR:HA	1:E:151:LEU:CD1	2.50	0.42
1:F:218:ALA:O	1:F:219:GLU:C	2.58	0.42
1:A:76:ILE:HD13	1:A:76:ILE:H	1.85	0.41
1:B:112:ARG:H	1:B:164:LEU:HD21	1.85	0.41
1:B:328:ILE:H	1:B:328:ILE:CD1	2.26	0.41
1:D:225:LEU:H	1:D:225:LEU:CD1	2.33	0.41
1:D:238:ASP:HA	1:D:239:SER:HA	1.68	0.41
1:F:142:SER:C	1:F:323:ARG:HD2	2.40	0.41
1:A:104:LEU:HD23	1:A:105:LYS:HD2	2.02	0.41
1:A:171:ILE:HD11	1:G:97:PHE:CE1	2.54	0.41
1:A:317:LYS:HG3	1:A:323:ARG:CZ	2.45	0.41
1:B:147:LEU:HA	1:B:347:ILE:HD11	2.01	0.41
1:B:171:ILE:HD12	1:B:214:LEU:HB3	2.02	0.41
1:C:179:PRO:HB2	1:C:197:LEU:HD11	2.01	0.41
1:C:243:HIS:O	1:C:247:GLU:HG3	2.21	0.41
1:C:285:VAL:O	1:C:286:GLN:HB2	2.20	0.41
1:E:219:GLU:CD	1:E:270:ARG:HH22	2.20	0.41
1:E:329:ASP:CG	1:E:330:ALA:N	2.74	0.41
1:E:332:HIS:O	1:E:333:LEU:HB2	2.19	0.41
1:G:189:ARG:HE	1:G:345:LYS:HB3	1.85	0.41
1:G:333:LEU:CB	1:G:334:PRO:HD2	2.50	0.41
1:B:322:LYS:HZ3	1:B:341:SER:HB3	1.86	0.41
1:C:100:ALA:HB2	1:D:200:ILE:HB	2.03	0.41
1:C:115:THR:HA	1:C:151:LEU:CD1	2.50	0.41
1:D:175:ASN:H	1:D:204:ARG:NH1	2.18	0.41
1:E:119:SER:CB	1:E:349:ASP:OD1	2.67	0.41
1:E:229:ASP:O	1:E:231:PRO:HD3	2.20	0.41
1:F:146:GLN:HE21	1:F:146:GLN:CA	2.21	0.41
1:F:181:ARG:O	1:F:185:ILE:HG13	2.20	0.41
1:A:62:ILE:HG23	1:A:70:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ARG:HG2	1:A:230:ARG:HH11	1.86	0.41
1:B:105:LYS:O	1:B:108:ALA:HB3	2.21	0.41
1:B:113:ILE:HD13	1:B:113:ILE:N	2.34	0.41
1:E:113:ILE:HD11	1:E:164:LEU:CD1	2.51	0.41
1:A:37:ILE:HD13	6:A:430:HOH:O	2.20	0.41
1:A:147:LEU:HD23	1:A:147:LEU:O	2.21	0.41
1:A:258:GLN:CG	1:B:249:ILE:CD1	2.96	0.41
1:D:207:ASN:N	1:D:243:HIS:CE1	2.89	0.41
1:E:213:LEU:HD13	1:E:217:GLN:OE1	2.20	0.41
1:F:113:ILE:CD1	1:F:164:LEU:CD1	2.98	0.41
1:G:305:LEU:HG	1:G:307:HIS:N	2.34	0.41
1:G:329:ASP:O	1:G:330:ALA:CB	2.68	0.41
1:D:187:GLN:CD	1:D:193:PRO:HG3	2.40	0.41
1:D:323:ARG:HG3	1:D:323:ARG:HH11	1.85	0.41
1:E:157:LEU:O	1:E:163:GLY:HA3	2.20	0.41
1:F:170:TRP:HB3	1:F:202:VAL:HG13	2.02	0.41
1:A:348:GLU:O	1:A:349:ASP:CB	2.69	0.41
1:B:221:LYS:HE2	1:B:225:LEU:CD2	2.51	0.41
1:E:147:LEU:HD22	1:E:151:LEU:HD22	2.02	0.41
1:F:147:LEU:CA	1:F:347:ILE:HD11	2.50	0.41
1:F:258:GLN:HG3	1:G:249:ILE:HD12	2.01	0.41
1:G:147:LEU:HD22	1:G:151:LEU:HD22	2.02	0.41
1:G:182:ILE:O	1:G:185:ILE:HG23	2.20	0.41
1:A:142:SER:HB2	1:A:315:LEU:HD12	2.02	0.41
1:A:209:ASN:O	1:A:213:LEU:HB2	2.20	0.41
1:C:170:TRP:HB3	1:C:202:VAL:HG13	1.98	0.41
1:F:238:ASP:HA	1:F:239:SER:HA	1.73	0.41
1:G:120:LEU:O	1:G:121:ASP:C	2.59	0.41
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.92	0.41
1:B:254:LEU:HD21	1:C:249:ILE:CG2	2.51	0.41
1:C:131:GLN:HA	1:C:272:ALA:O	2.21	0.41
1:C:265:LEU:HD21	1:C:306:ALA:HA	2.03	0.41
1:D:97:PHE:CD2	1:E:203:ALA:HB2	2.55	0.41
1:D:154:MSE:O	1:D:157:LEU:HG	2.19	0.41
1:D:186:ALA:C	1:D:188:ASN:H	2.24	0.41
1:D:187:GLN:HG3	1:D:187:GLN:O	2.21	0.41
1:F:265:LEU:HD12	1:F:265:LEU:HA	1.89	0.41
1:F:316:ARG:HG2	1:F:324:ILE:CG2	2.51	0.41
1:G:116:GLY:O	1:G:348:GLU:HA	2.21	0.41
1:G:156:GLN:HE21	1:G:196:VAL:HG13	1.81	0.41
1:G:158:PRO:HA	1:G:159:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:VAL:HB	1:G:281:VAL:HG12	2.02	0.41
1:G:314:TYR:CB	1:G:328:ILE:HD11	2.50	0.41
1:B:348:GLU:OE2	1:B:348:GLU:O	2.39	0.41
1:C:187:GLN:HB3	1:C:193:PRO:CG	2.50	0.41
1:C:286:GLN:NE2	1:C:286:GLN:CA	2.82	0.41
1:E:221:LYS:HD2	1:E:221:LYS:HA	1.86	0.41
1:G:120:LEU:HD22	1:G:124:LEU:HD12	2.03	0.41
1:G:122:LYS:C	1:G:124:LEU:N	2.74	0.41
1:G:122:LYS:O	1:G:124:LEU:N	2.53	0.41
1:D:100:ALA:HB3	1:E:197:LEU:O	2.21	0.40
1:D:308:SER:HB3	1:D:309:ALA:H	1.72	0.40
1:D:323:ARG:HD3	1:D:342:ILE:HD11	2.04	0.40
1:G:184:GLU:O	1:G:186:ALA:N	2.54	0.40
1:A:170:TRP:CE3	1:A:236:ILE:HD12	2.56	0.40
1:A:344:GLU:CD	1:A:344:GLU:N	2.72	0.40
1:C:251:ARG:HH21	1:D:251:ARG:CA	2.25	0.40
1:D:136:VAL:O	1:D:136:VAL:HG13	2.21	0.40
1:D:158:PRO:HD2	1:D:161:GLU:OE2	2.21	0.40
1:F:192:ASP:HA	1:F:193:PRO:HD2	1.96	0.40
1:F:219:GLU:O	1:F:219:GLU:HG3	2.20	0.40
1:G:166:GLY:HA3	1:G:233:LYS:HG3	2.02	0.40
1:A:136:VAL:O	1:A:136:VAL:HG13	2.21	0.40
1:A:183:ARG:HE	1:A:193:PRO:HB2	1.87	0.40
1:D:195:GLU:O	1:D:198:LYS:HB2	2.22	0.40
1:E:205:ALA:O	1:E:243:HIS:HE1	2.03	0.40
1:G:122:LYS:C	1:G:124:LEU:H	2.25	0.40
1:G:183:ARG:HH22	1:G:194:ASP:CG	2.23	0.40
1:D:147:LEU:HA	1:D:347:ILE:CD1	2.52	0.40
1:D:147:LEU:HG	1:D:347:ILE:CD1	2.52	0.40
1:E:140:PHE:HB2	1:E:284:GLN:OE1	2.21	0.40
1:G:212:MSE:HE1	1:G:260:LYS:HD3	2.03	0.40
1:G:261:LEU:HD13	1:G:304:ILE:HD11	2.04	0.40
1:A:60:GLU:HA	1:A:63:ALA:HB3	2.03	0.40
1:A:179:PRO:HD2	1:A:180:GLU:OE1	2.21	0.40
1:A:184:GLU:O	1:A:185:ILE:C	2.60	0.40
1:E:156:GLN:HE21	1:E:196:VAL:HG13	1.79	0.40
1:E:318:GLY:O	1:E:319:LYS:O	2.39	0.40
1:F:157:LEU:HD13	1:F:161:GLU:HB2	2.03	0.40
1:F:207:ASN:N	1:F:243:HIS:CE1	2.90	0.40
1:G:225:LEU:HD12	1:G:225: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	296/349 (85%)	265 (90%)	20 (7%)	11 (4%)	3 11
1	B	235/349 (67%)	203 (86%)	25 (11%)	7 (3%)	4 14
1	C	235/349 (67%)	199 (85%)	25 (11%)	11 (5%)	2 7
1	D	235/349 (67%)	199 (85%)	26 (11%)	10 (4%)	2 8
1	E	235/349 (67%)	212 (90%)	15 (6%)	8 (3%)	3 12
1	F	235/349 (67%)	207 (88%)	23 (10%)	5 (2%)	7 22
1	G	234/349 (67%)	187 (80%)	31 (13%)	16 (7%)	1 2
All	All	1705/2443 (70%)	1472 (86%)	165 (10%)	68 (4%)	3 9

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PRO
1	A	319	LYS
1	A	334	PRO
1	B	329	ASP
1	B	330	ALA
1	C	329	ASP
1	C	330	ALA
1	D	191	LEU
1	D	319	LYS
1	D	329	ASP
1	D	330	ALA
1	E	303	HIS
1	E	319	LYS
1	E	329	ASP
1	E	330	ALA
1	E	334	PRO
1	F	319	LYS
1	G	184	GLU

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Mol	Chain	Res	Type
1	G	191	LEU
1	G	197	LEU
1	G	225	LEU
1	G	330	ALA
1	G	333	LEU
1	G	334	PRO
1	A	184	GLU
1	A	185	ILE
1	B	252	GLY
1	B	319	LYS
1	C	197	LEU
1	C	225	LEU
1	C	253	ALA
1	D	250	GLY
1	D	308	SER
1	E	332	HIS
1	F	219	GLU
1	G	185	ILE
1	G	224	GLU
1	G	329	ASP
1	A	303	HIS
1	A	329	ASP
1	B	188	ASN
1	C	186	ALA
1	C	224	GLU
1	C	319	LYS
1	D	184	GLU
1	D	186	ALA
1	F	197	LEU
1	F	332	HIS
1	G	193	PRO
1	G	223	LYS
1	G	326	ARG
1	C	188	ASN
1	D	197	LEU
1	G	123	LEU
1	D	164	LEU
1	E	253	ALA
1	E	333	LEU
1	G	122	LYS
1	G	307	HIS
1	A	37	ILE

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Mol	Chain	Res	Type
1	A	330	ALA
1	A	333	LEU
1	C	334	PRO
1	A	192	ASP
1	B	333	LEU
1	B	334	PRO
1	C	333	LEU
1	F	334	PRO

5.3.2 Protein sidechains (i)

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	242/279 (87%)	217 (90%)	25 (10%)	7	19
1	B	199/279 (71%)	176 (88%)	23 (12%)	5	14
1	C	199/279 (71%)	180 (90%)	19 (10%)	8	23
1	D	199/279 (71%)	175 (88%)	24 (12%)	5	13
1	E	199/279 (71%)	179 (90%)	20 (10%)	7	20
1	F	199/279 (71%)	175 (88%)	24 (12%)	5	13
1	G	199/279 (71%)	179 (90%)	20 (10%)	7	20
All	All	1436/1953 (74%)	1281 (89%)	155 (11%)	6	17

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	37	ILE
1	A	41	PRO
1	A	64	VAL
1	A	76	ILE
1	A	93	ASN
1	A	94	LEU
1	A	102	GLU
1	A	104	LEU

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Mol	Chain	Res	Type
1	A	107	ARG
1	A	112	ARG
1	A	121	ASP
1	A	129	GLU
1	A	147	LEU
1	A	151	LEU
1	A	187	GLN
1	A	202	VAL
1	A	254	LEU
1	A	265	LEU
1	A	274	LEU
1	A	283	ASN
1	A	305	LEU
1	A	323	ARG
1	A	324	ILE
1	A	342	ILE
1	B	120	LEU
1	B	121	ASP
1	B	129	GLU
1	B	151	LEU
1	B	160	GLU
1	B	182	ILE
1	B	194	ASP
1	B	202	VAL
1	B	220	ASP
1	B	225	LEU
1	B	229	ASP
1	B	249	ILE
1	B	251	ARG
1	B	261	LEU
1	B	265	LEU
1	B	274	LEU
1	B	283	ASN
1	B	304	ILE
1	B	323	ARG
1	B	329	ASP
1	B	332	HIS
1	B	342	ILE
1	B	348	GLU
1	C	99	ARG
1	C	104	LEU
1	C	112	ARG

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Mol	Chain	Res	Type
1	C	129	GLU
1	C	151	LEU
1	C	188	ASN
1	C	191	LEU
1	C	197	LEU
1	C	202	VAL
1	C	216	GLN
1	C	224	GLU
1	C	263	LYS
1	C	265	LEU
1	C	274	LEU
1	C	283	ASN
1	C	307	HIS
1	C	327	LEU
1	C	342	ILE
1	C	348	GLU
1	D	105	LYS
1	D	112	ARG
1	D	120	LEU
1	D	129	GLU
1	D	151	LEU
1	D	188	ASN
1	D	196	VAL
1	D	202	VAL
1	D	204	ARG
1	D	213	LEU
1	D	222	ILE
1	D	224	GLU
1	D	259	GLN
1	D	263	LYS
1	D	265	LEU
1	D	274	LEU
1	D	283	ASN
1	D	286	GLN
1	D	305	LEU
1	D	323	ARG
1	D	324	ILE
1	D	326	ARG
1	D	332	HIS
1	D	342	ILE
1	E	104	LEU
1	E	112	ARG

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Mol	Chain	Res	Type
1	E	120	LEU
1	E	121	ASP
1	E	129	GLU
1	E	151	LEU
1	E	188	ASN
1	E	202	VAL
1	E	251	ARG
1	E	257	ARG
1	E	261	LEU
1	E	263	LYS
1	E	265	LEU
1	E	274	LEU
1	E	283	ASN
1	E	304	ILE
1	E	305	LEU
1	E	324	ILE
1	E	332	HIS
1	E	349	ASP
1	F	99	ARG
1	F	105	LYS
1	F	109	THR
1	F	112	ARG
1	F	117	SER
1	F	121	ASP
1	F	129	GLU
1	F	151	LEU
1	F	201	TYR
1	F	202	VAL
1	F	213	LEU
1	F	214	LEU
1	F	251	ARG
1	F	258	GLN
1	F	261	LEU
1	F	265	LEU
1	F	274	LEU
1	F	283	ASN
1	F	286	GLN
1	F	307	HIS
1	F	324	ILE
1	F	329	ASP
1	F	332	HIS
1	F	342	ILE

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Mol	Chain	Res	Type
1	G	97	PHE
1	G	99	ARG
1	G	124	LEU
1	G	129	GLU
1	G	151	LEU
1	G	160	GLU
1	G	185	ILE
1	G	194	ASP
1	G	202	VAL
1	G	229	ASP
1	G	245	ARG
1	G	261	LEU
1	G	265	LEU
1	G	274	LEU
1	G	283	ASN
1	G	286	GLN
1	G	305	LEU
1	G	324	ILE
1	G	342	ILE
1	G	349	ASP

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

Mol	Chain	Res	Type
1	A	86	GLN
1	A	93	ASN
1	A	146	GLN
1	A	165	ASN
1	A	187	GLN
1	A	188	ASN
1	A	199	HIS
1	A	216	GLN
1	A	243	HIS
1	A	259	GLN
1	A	264	HIS
1	A	273	ASN
1	A	283	ASN
1	A	286	GLN
1	B	146	GLN
1	B	165	ASN
1	B	243	HIS
1	B	264	HIS

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Mol	Chain	Res	Type
1	B	273	ASN
1	B	283	ASN
1	C	146	GLN
1	C	165	ASN
1	C	187	GLN
1	C	264	HIS
1	C	273	ASN
1	C	283	ASN
1	C	286	GLN
1	D	146	GLN
1	D	165	ASN
1	D	187	GLN
1	D	199	HIS
1	D	264	HIS
1	D	273	ASN
1	D	283	ASN
1	D	286	GLN
1	D	303	HIS
1	E	146	GLN
1	E	165	ASN
1	E	264	HIS
1	E	273	ASN
1	E	283	ASN
1	E	286	GLN
1	E	303	HIS
1	F	146	GLN
1	F	165	ASN
1	F	211	GLN
1	F	227	ASN
1	F	258	GLN
1	F	273	ASN
1	F	283	ASN
1	F	286	GLN
1	F	332	HIS
1	G	146	GLN
1	G	165	ASN
1	G	187	GLN
1	G	211	GLN
1	G	227	ASN
1	G	273	ASN
1	G	283	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

29 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	$\#\|Z\| > 2$
2	SO4	A	350	-	4,4,4	0.25	0	6,6,6	0.65	0
2	SO4	G	356	-	4,4,4	0.44	0	6,6,6	0.56	0
3	IMD	B	360	-	3,5,5	0.79	0	4,5,5	0.57	0
4	GOL	F	372	-	5,5,5	4.56	5 (100%)	5,5,5	5.74	3 (60%)
4	GOL	F	366	-	5,5,5	4.70	5 (100%)	5,5,5	5.78	3 (60%)
4	GOL	A	374	-	5,5,5	4.54	5 (100%)	5,5,5	5.60	3 (60%)
3	IMD	A	357	-	3,5,5	0.61	0	4,5,5	0.48	0
3	IMD	F	363	-	3,5,5	0.74	0	4,5,5	0.35	0
4	GOL	C	370	-	5,5,5	4.39	4 (80%)	5,5,5	5.64	3 (60%)
3	IMD	B	359	-	3,5,5	0.61	0	4,5,5	0.46	0
4	GOL	E	371	-	5,5,5	4.65	5 (100%)	5,5,5	5.69	3 (60%)
4	GOL	D	369	-	5,5,5	4.73	5 (100%)	5,5,5	5.82	3 (60%)
4	GOL	F	373	-	5,5,5	4.39	5 (100%)	5,5,5	5.82	3 (60%)
3	IMD	A	361	-	3,5,5	0.89	0	4,5,5	0.55	0
3	IMD	C	362	-	3,5,5	1.00	0	4,5,5	0.52	0
2	SO4	F	355	-	4,4,4	0.35	0	6,6,6	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	IMD	A	364	-	3,5,5	0.92	0	4,5,5	0.51	0
4	GOL	B	367	-	5,5,5	4.47	5 (100%)	5,5,5	5.72	3 (60%)
3	IMD	A	358	-	3,5,5	0.73	0	4,5,5	0.48	0
2	SO4	B	351	-	4,4,4	0.38	0	6,6,6	0.80	0
5	MPD	E	376	-	7,7,7	0.69	0	9,10,10	0.62	0
4	GOL	C	368	-	5,5,5	4.54	5 (100%)	5,5,5	5.70	3 (60%)
2	SO4	D	353	-	4,4,4	0.37	0	6,6,6	0.72	0
5	MPD	B	375	-	7,7,7	0.62	0	9,10,10	0.56	0
5	MPD	G	378	-	7,7,7	0.73	0	9,10,10	0.51	0
5	MPD	G	377	-	7,7,7	0.68	0	9,10,10	0.53	0
2	SO4	C	352	-	4,4,4	0.44	0	6,6,6	0.70	0
3	IMD	B	365	-	3,5,5	0.90	0	4,5,5	0.59	0
2	SO4	E	354	-	4,4,4	0.29	0	6,6,6	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMD	B	360	-	-	-	0/1/1/1
4	GOL	F	372	-	-	3/4/4/4	-
4	GOL	F	366	-	-	2/4/4/4	-
4	GOL	A	374	-	-	3/4/4/4	-
3	IMD	A	357	-	-	-	0/1/1/1
4	GOL	C	370	-	-	2/4/4/4	-
4	GOL	E	371	-	-	2/4/4/4	-
3	IMD	B	359	-	-	-	0/1/1/1
3	IMD	F	363	-	-	-	0/1/1/1
4	GOL	D	369	-	-	3/4/4/4	-
4	GOL	F	373	-	-	2/4/4/4	-
3	IMD	A	361	-	-	-	0/1/1/1
3	IMD	C	362	-	-	-	0/1/1/1
3	IMD	A	364	-	-	-	0/1/1/1
4	GOL	B	367	-	-	2/4/4/4	-
3	IMD	A	358	-	-	-	0/1/1/1
5	MPD	E	376	-	-	1/5/5/5	-
4	GOL	C	368	-	-	3/4/4/4	-
5	MPD	B	375	-	-	0/5/5/5	-
5	MPD	G	378	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	G	377	-	-	0/5/5/5	-
3	IMD	B	365	-	-	-	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	366	GOL	C3-C2	-7.65	1.20	1.51
4	E	371	GOL	C3-C2	-7.58	1.20	1.51
4	C	368	GOL	C3-C2	-7.37	1.21	1.51
4	B	367	GOL	C3-C2	-7.33	1.21	1.51
4	A	374	GOL	C3-C2	-7.31	1.21	1.51
4	D	369	GOL	C3-C2	-7.27	1.21	1.51
4	C	370	GOL	C3-C2	-7.20	1.22	1.51
4	F	372	GOL	C3-C2	-7.15	1.22	1.51
4	F	373	GOL	C3-C2	-6.91	1.23	1.51
4	F	373	GOL	O1-C1	5.48	1.65	1.42
4	D	369	GOL	O1-C1	5.18	1.64	1.42
4	C	370	GOL	O1-C1	4.82	1.62	1.42
4	F	372	GOL	O1-C1	4.81	1.62	1.42
4	A	374	GOL	O1-C1	4.70	1.62	1.42
4	E	371	GOL	O1-C1	4.70	1.62	1.42
4	F	366	GOL	O1-C1	4.60	1.61	1.42
4	C	368	GOL	O1-C1	4.47	1.61	1.42
4	B	367	GOL	O1-C1	4.36	1.60	1.42
4	D	369	GOL	O2-C2	-3.83	1.32	1.43
4	B	367	GOL	O3-C3	3.71	1.58	1.42
4	A	374	GOL	O3-C3	3.61	1.57	1.42
4	F	366	GOL	O2-C2	-3.54	1.32	1.43
4	F	372	GOL	O3-C3	3.49	1.57	1.42
4	C	368	GOL	O3-C3	3.34	1.56	1.42
4	C	370	GOL	O3-C3	3.32	1.56	1.42
4	E	371	GOL	O3-C3	3.24	1.56	1.42
4	E	371	GOL	C1-C2	-3.24	1.38	1.51
4	D	369	GOL	O3-C3	3.21	1.56	1.42
4	F	372	GOL	C1-C2	-3.21	1.38	1.51
4	A	374	GOL	C1-C2	-3.19	1.38	1.51
4	C	368	GOL	C1-C2	-3.14	1.38	1.51
4	F	366	GOL	C1-C2	-3.06	1.39	1.51
4	F	373	GOL	O3-C3	3.03	1.55	1.42
4	F	366	GOL	O3-C3	2.95	1.54	1.42
4	C	368	GOL	O2-C2	-2.77	1.35	1.43
4	E	371	GOL	O2-C2	-2.75	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	369	GOL	C1-C2	-2.69	1.40	1.51
4	B	367	GOL	O2-C2	-2.68	1.35	1.43
4	F	372	GOL	O2-C2	-2.66	1.35	1.43
4	C	370	GOL	C1-C2	-2.56	1.41	1.51
4	B	367	GOL	C1-C2	-2.52	1.41	1.51
4	F	373	GOL	C1-C2	-2.31	1.42	1.51
4	A	374	GOL	O2-C2	-2.13	1.37	1.43
4	F	373	GOL	O2-C2	-2.02	1.37	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	373	GOL	O3-C3-C2	10.71	161.54	110.20
4	D	369	GOL	O3-C3-C2	10.51	160.61	110.20
4	F	366	GOL	O3-C3-C2	10.42	160.14	110.20
4	E	371	GOL	O3-C3-C2	10.38	159.98	110.20
4	C	368	GOL	O3-C3-C2	10.33	159.73	110.20
4	F	372	GOL	O3-C3-C2	10.33	159.72	110.20
4	B	367	GOL	O3-C3-C2	10.31	159.65	110.20
4	A	374	GOL	O3-C3-C2	10.28	159.50	110.20
4	C	370	GOL	O3-C3-C2	10.11	158.66	110.20
4	F	372	GOL	O2-C2-C3	7.00	139.93	109.12
4	D	369	GOL	O2-C2-C3	6.79	139.04	109.12
4	F	366	GOL	O2-C2-C3	6.79	139.02	109.12
4	C	370	GOL	O2-C2-C3	6.78	138.98	109.12
4	B	367	GOL	O2-C2-C3	6.71	138.66	109.12
4	C	368	GOL	O2-C2-C3	6.70	138.65	109.12
4	A	374	GOL	O2-C2-C3	6.69	138.59	109.12
4	E	371	GOL	O2-C2-C3	6.69	138.57	109.12
4	F	373	GOL	O2-C2-C3	6.50	137.74	109.12
4	D	369	GOL	O1-C1-C2	3.47	126.86	110.20
4	F	366	GOL	O1-C1-C2	3.38	126.41	110.20
4	B	367	GOL	O1-C1-C2	3.34	126.23	110.20
4	F	373	GOL	O1-C1-C2	3.29	125.98	110.20
4	C	368	GOL	O1-C1-C2	3.22	125.66	110.20
4	C	370	GOL	O1-C1-C2	3.10	125.05	110.20
4	F	372	GOL	O1-C1-C2	2.93	124.25	110.20
4	E	371	GOL	O1-C1-C2	2.91	124.16	110.20
4	A	374	GOL	O1-C1-C2	2.43	121.87	110.20

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	374	GOL	O1-C1-C2-C3
4	A	374	GOL	C1-C2-C3-O3
4	B	367	GOL	C1-C2-C3-O3
4	C	368	GOL	O1-C1-C2-C3
4	C	368	GOL	C1-C2-C3-O3
4	C	370	GOL	C1-C2-C3-O3
4	D	369	GOL	O1-C1-C2-C3
4	D	369	GOL	C1-C2-C3-O3
4	E	371	GOL	C1-C2-C3-O3
4	F	366	GOL	O1-C1-C2-C3
4	F	366	GOL	C1-C2-C3-O3
4	F	372	GOL	C1-C2-C3-O3
4	F	373	GOL	O1-C1-C2-O2
4	F	373	GOL	C1-C2-C3-O3
4	B	367	GOL	O1-C1-C2-O2
4	C	370	GOL	O1-C1-C2-O2
4	E	371	GOL	O1-C1-C2-O2
4	A	374	GOL	O1-C1-C2-O2
4	C	368	GOL	O1-C1-C2-O2
4	F	372	GOL	O1-C1-C2-O2
4	F	372	GOL	O1-C1-C2-C3
5	E	376	MPD	C1-C2-C3-C4
4	D	369	GOL	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	SO4	1	0
2	G	356	SO4	1	0
3	B	360	IMD	2	0
3	F	363	IMD	3	0
3	B	359	IMD	6	0
4	D	369	GOL	2	0
4	F	373	GOL	2	0
3	A	361	IMD	2	0
2	F	355	SO4	1	0
4	B	367	GOL	1	0
4	C	368	GOL	1	0
2	C	352	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	297/349 (85%)	-0.11	5 (1%)	70	68	28, 66, 110, 161	0
1	B	236/349 (67%)	0.13	5 (2%)	63	60	32, 74, 132, 170	0
1	C	236/349 (67%)	0.18	18 (7%)	13	10	39, 78, 137, 198	0
1	D	236/349 (67%)	0.29	14 (5%)	22	17	41, 86, 139, 175	0
1	E	236/349 (67%)	0.04	9 (3%)	40	35	30, 62, 116, 197	0
1	F	236/349 (67%)	0.09	7 (2%)	50	45	37, 75, 121, 177	0
1	G	235/349 (67%)	0.20	17 (7%)	15	11	41, 82, 138, 190	0
All	All	1712/2443 (70%)	0.11	75 (4%)	34	29	28, 74, 133, 198	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	345	LYS	6.2
1	C	333	LEU	4.6
1	D	302	GLY	4.5
1	G	250	GLY	4.2
1	G	349	ASP	4.2
1	E	302	GLY	3.8
1	C	250	GLY	3.7
1	G	332	HIS	3.6
1	D	349	ASP	3.6
1	D	338	ALA	3.5
1	G	337	GLU	3.4
1	D	348	GLU	3.4
1	D	333	LEU	3.3
1	B	349	ASP	3.3
1	C	227	ASN	3.3
1	E	250	GLY	3.2
1	E	249	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	334	PRO	3.2
1	D	345	LYS	3.2
1	G	339	VAL	3.2
1	G	340	PHE	3.2
1	E	331	PRO	3.1
1	E	304	ILE	3.1
1	F	335	GLU	3.0
1	B	194	ASP	3.0
1	E	349	ASP	2.9
1	D	162	GLY	2.9
1	C	331	PRO	2.8
1	C	319	LYS	2.8
1	C	335	GLU	2.8
1	C	303	HIS	2.8
1	A	250	GLY	2.7
1	G	221	LYS	2.7
1	G	314	TYR	2.7
1	G	319	LYS	2.7
1	G	338	ALA	2.7
1	G	276	ASP	2.6
1	E	303	HIS	2.6
1	F	250	GLY	2.6
1	A	35	ARG	2.6
1	C	218	ALA	2.5
1	F	349	ASP	2.5
1	G	224	GLU	2.5
1	D	226	LEU	2.5
1	A	161	GLU	2.5
1	E	190	GLY	2.5
1	G	227	ASN	2.5
1	C	343	THR	2.5
1	C	339	VAL	2.4
1	G	333	LEU	2.4
1	C	276	ASP	2.4
1	F	249	ILE	2.4
1	E	227	ASN	2.4
1	C	302	GLY	2.4
1	C	323	ARG	2.3
1	A	307	HIS	2.3
1	C	348	GLU	2.3
1	B	303	HIS	2.3
1	D	324	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	225	LEU	2.2
1	G	326	ARG	2.2
1	A	349	ASP	2.2
1	D	332	HIS	2.2
1	B	345	LYS	2.2
1	C	318	GLY	2.2
1	F	338	ALA	2.1
1	C	345	LYS	2.1
1	F	302	GLY	2.1
1	D	342	ILE	2.1
1	C	186	ALA	2.1
1	B	338	ALA	2.1
1	D	339	VAL	2.0
1	G	327	LEU	2.0
1	D	322	LYS	2.0
1	D	314	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IMD	A	361	5/5	0.71	0.23	119,119,119,119	0
3	IMD	F	363	5/5	0.73	0.42	100,100,100,100	0
4	GOL	B	367	6/6	0.82	0.14	68,68,68,68	0
4	GOL	D	369	6/6	0.83	0.27	79,79,79,79	0
5	MPD	G	377	8/8	0.84	0.24	106,106,106,106	0
5	MPD	G	378	8/8	0.84	0.48	112,112,112,112	0
5	MPD	E	376	8/8	0.85	0.23	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IMD	A	358	5/5	0.86	0.17	101,101,101,101	0
3	IMD	C	362	5/5	0.86	0.35	94,94,94,94	0
4	GOL	C	368	6/6	0.86	0.13	77,77,77,77	0
4	GOL	C	370	6/6	0.86	0.13	88,88,88,88	0
4	GOL	E	371	6/6	0.89	0.15	66,66,66,66	0
3	IMD	B	365	5/5	0.89	0.12	92,92,92,92	0
4	GOL	A	374	6/6	0.90	0.22	76,76,76,76	0
3	IMD	B	360	5/5	0.90	0.14	81,81,81,81	0
3	IMD	B	359	5/5	0.90	0.15	76,76,76,76	0
2	SO4	F	355	5/5	0.91	0.20	91,91,91,91	0
3	IMD	A	364	5/5	0.91	0.16	93,93,93,93	0
5	MPD	B	375	8/8	0.94	0.23	53,53,53,53	0
4	GOL	F	366	6/6	0.94	0.22	66,66,66,66	0
4	GOL	F	372	6/6	0.94	0.20	76,76,76,76	0
4	GOL	F	373	6/6	0.94	0.22	88,88,88,88	0
3	IMD	A	357	5/5	0.96	0.08	90,90,90,90	0
2	SO4	C	352	5/5	0.96	0.11	71,71,71,71	0
2	SO4	B	351	5/5	0.97	0.15	65,65,65,65	0
2	SO4	G	356	5/5	0.97	0.10	66,66,66,66	0
2	SO4	D	353	5/5	0.97	0.10	78,78,78,78	0
2	SO4	E	354	5/5	0.97	0.14	60,60,60,60	0
2	SO4	A	350	5/5	0.98	0.14	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.