



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:02 AM UTC

PDB ID : 4XRP / pdb_00004xrp
Title : Structure of the Pnkp1/Rnl/Hen1 RNA repair complex
Authors : Huang, R.H.; Wang, P.
Deposited on : 2015-01-21
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

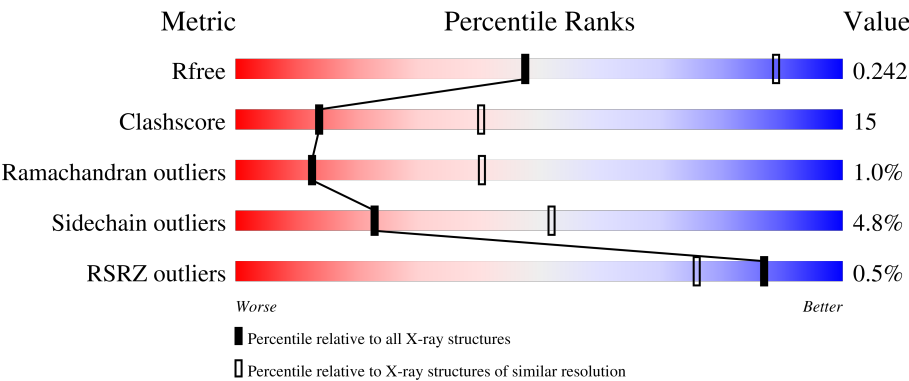
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	312	60%35%. .
1	D	312	% 51%42%6%. .
2	B	394	66%32%. .
2	E	394	66%31%. .
3	C	436	% 63%29%. . .

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Mol	Chain	Length	Quality of chain
3	F	436	% 64% 29% ...

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
4	PO4	A	401	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18888 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 Pnkp1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2544	1620	433	479	12			
1	D	311	Total	C	N	O	S	0	0	0
			2544	1620	433	479	12			

- Molecule 2 is a protein called Rnl.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	0	0
			3289	2116	557	607	9			
2	E	393	Total	C	N	O	S	0	0	0
			3281	2111	556	606	8			

- Molecule 3 is a protein called Hen1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	424	Total	C	N	O	S	0	0	0
			3537	2286	580	654	17			
3	F	422	Total	C	N	O	S	0	0	0
			3516	2271	576	652	17			

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	2	Total	Mg	0	0
			2	2		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		

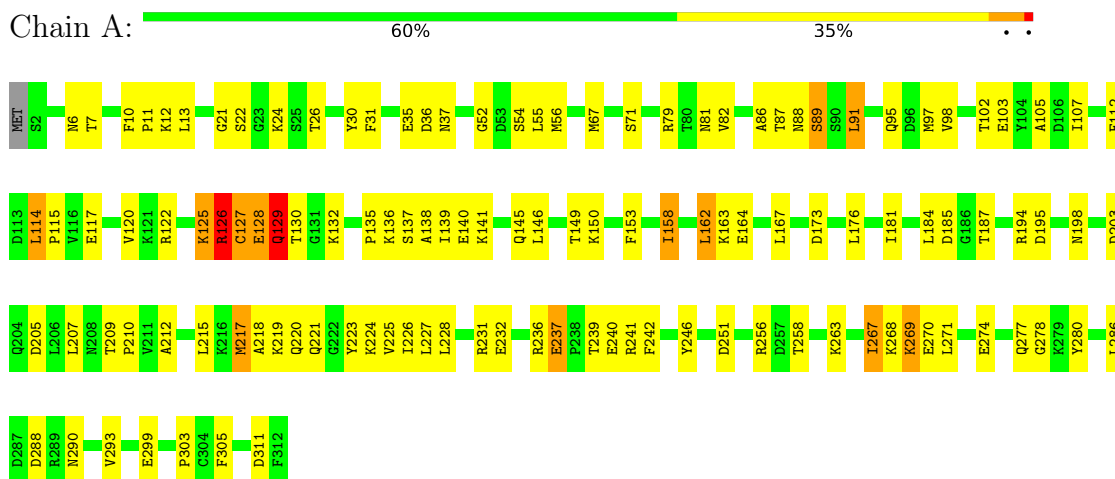
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	7	Total	O	0	0
			7	7		
8	B	18	Total	O	0	0
			18	18		
8	C	22	Total	O	0	0
			22	22		
8	D	9	Total	O	0	0
			9	9		
8	E	17	Total	O	0	0
			17	17		
8	F	20	Total	O	0	0
			20	20		

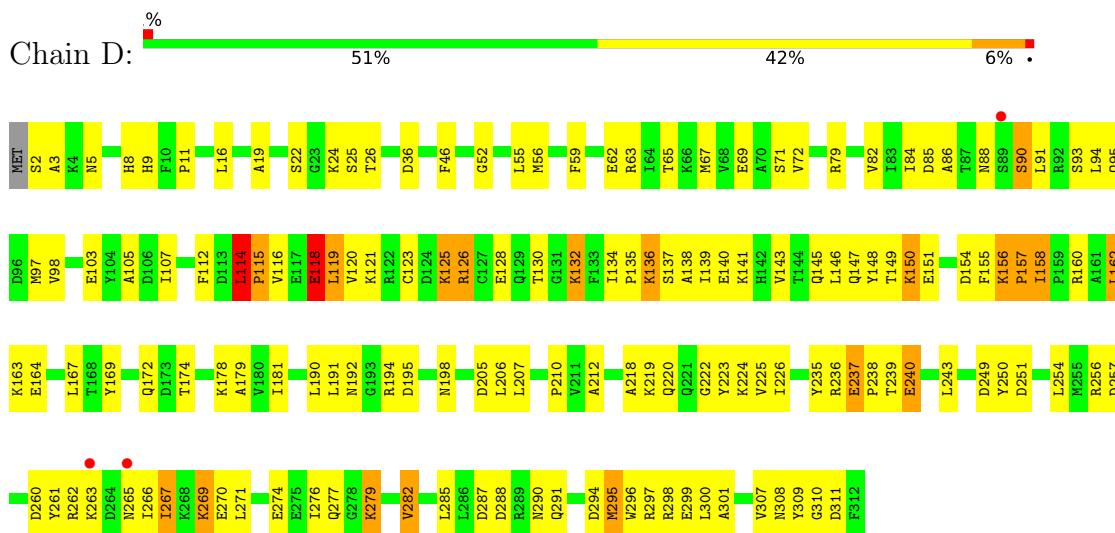
3 Residue-property plots

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

• Molecule 1: Pnkp1

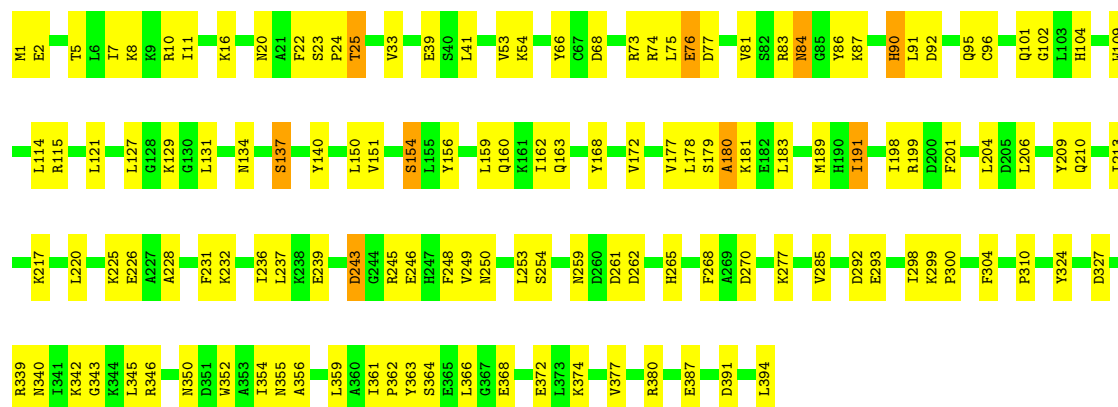


• Molecule 1: Pnkp1



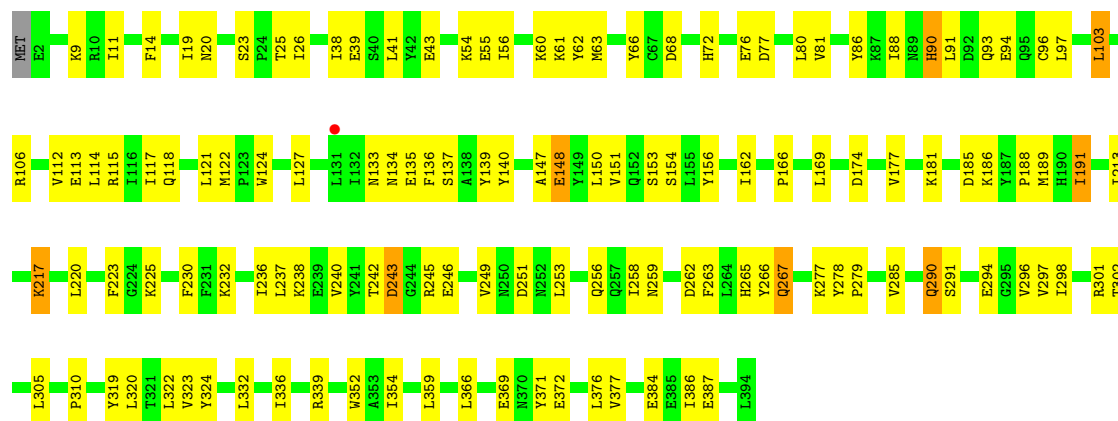
• Molecule 2: Rnl





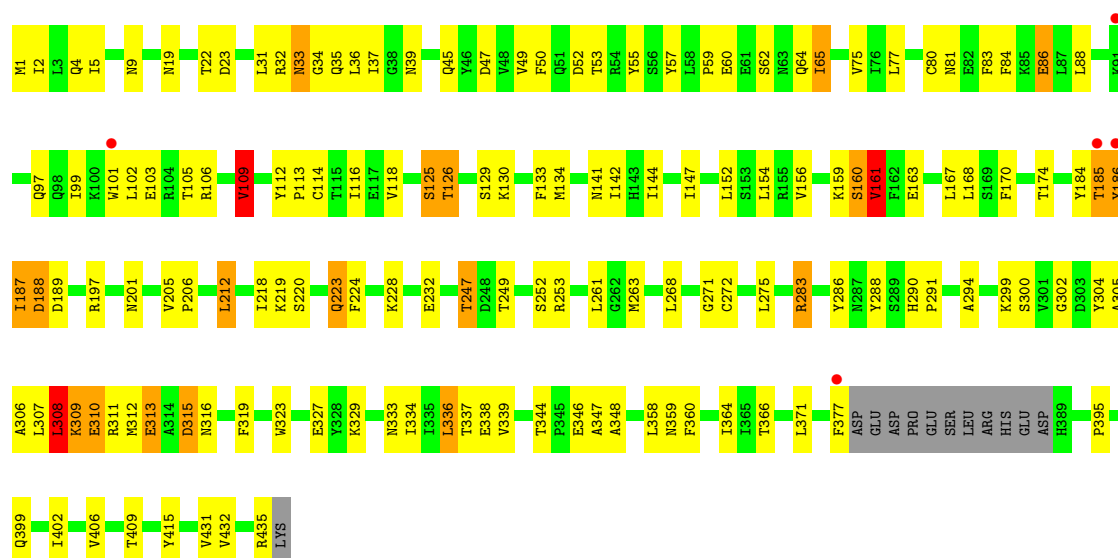
• Molecule 2: Rnl

Chain E: 66% 31% .

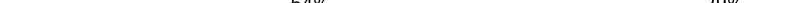


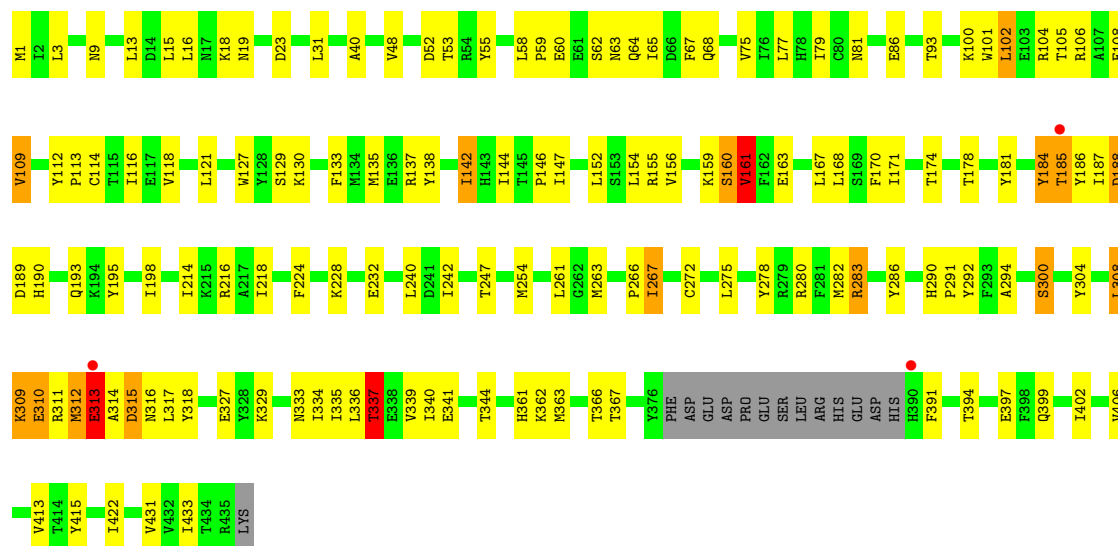
• Molecule 3: Hen1

Chain C: 63% 29% . . .



- Molecule 3: Hen1

Chain F:  %



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.16Å 179.20Å 114.33Å 90.00° 103.70° 90.00°	Depositor
Resolution (Å)	47.21 – 3.30 47.21 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.21-3.30) 96.8 (47.21-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1624)	Depositor
R, R_{free}	0.175 , 0.238 0.180 , 0.242	Depositor DCC
R_{free} test set	1991 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18888	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SO4, GOL, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.67	1/2594 (0.0%)	1.18	18/3501 (0.5%)
1	D	0.66	0/2594	1.22	18/3501 (0.5%)
2	B	0.73	0/3366	1.11	9/4544 (0.2%)
2	E	0.64	0/3358	1.06	8/4534 (0.2%)
3	C	0.71	1/3636 (0.0%)	1.12	21/4932 (0.4%)
3	F	0.72	0/3613	1.09	15/4901 (0.3%)
All	All	0.69	2/19161 (0.0%)	1.12	89/25913 (0.3%)

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	D	0	1
3	C	0	2
3	F	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	308	LEU	CA-C	6.78	1.61	1.53
1	A	129	GLN	CG-CD	5.59	1.66	1.52

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	310	GLU	N-CA-C	-12.98	96.82	113.17
1	A	237	GLU	CA-C-N	-11.29	107.84	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	GLU	C-N-CA	-11.29	107.84	120.04
3	C	33	ASN	N-CA-C	11.16	125.45	112.72
1	A	129	GLN	N-CA-C	10.06	127.87	111.37
3	C	252	SER	N-CA-C	-8.75	101.70	111.07
2	E	134	ASN	N-CA-C	-8.63	102.74	113.18
1	D	237	GLU	CA-C-N	-8.57	110.78	120.04
1	D	237	GLU	C-N-CA	-8.57	110.78	120.04
1	D	114	LEU	CA-C-N	8.55	128.61	119.89
1	D	114	LEU	C-N-CA	8.55	128.61	119.89
1	A	126	ARG	N-CA-C	-8.25	93.23	110.80
2	B	134	ASN	N-CA-C	-8.23	102.69	112.89
3	F	339	VAL	N-CA-C	-7.86	106.25	113.71
3	F	161	VAL	N-CA-C	-7.33	103.31	110.72
1	A	128	GLU	CA-C-N	7.26	132.74	121.19
1	A	128	GLU	C-N-CA	7.26	132.74	121.19
1	D	119	LEU	N-CA-C	-7.25	103.40	112.90
3	F	309	LYS	N-CA-C	-7.01	104.65	112.57
2	B	129	LYS	N-CA-C	-7.01	104.72	113.55
1	D	115	PRO	N-CA-C	6.90	122.08	111.11
1	D	136	LYS	N-CA-C	-6.85	105.33	113.21
1	D	126	ARG	CG-CD-NE	6.79	126.94	112.00
1	D	156	LYS	CA-C-N	6.76	126.78	119.89
1	D	156	LYS	C-N-CA	6.76	126.78	119.89
3	C	161	VAL	N-CA-C	-6.69	103.97	110.72
1	A	89	SER	N-CA-C	-6.57	106.47	114.75
1	D	157	PRO	N-CA-C	6.51	121.47	111.11
2	B	299	LYS	N-CA-C	-6.47	100.67	110.50
1	D	150	LYS	N-CA-C	-6.46	104.33	111.82
3	C	109	VAL	N-CA-C	6.37	117.06	111.90
3	F	344	THR	CA-C-N	6.29	126.49	119.32
3	F	344	THR	C-N-CA	6.29	126.49	119.32
3	F	300	SER	N-CA-C	-6.21	105.72	113.55
2	E	191	ILE	N-CA-C	-6.17	104.84	110.82
2	B	191	ILE	N-CA-C	-6.16	105.72	111.45
3	C	290	HIS	CA-C-N	-6.14	114.31	120.21
3	C	290	HIS	C-N-CA	-6.14	114.31	120.21
3	F	93	THR	N-CA-C	6.14	118.48	111.11
1	A	162	LEU	CA-C-N	-6.06	114.36	122.72
1	A	162	LEU	C-N-CA	-6.06	114.36	122.72
3	F	102	LEU	N-CA-C	-6.06	100.28	109.85
1	A	114	LEU	CA-C-N	6.01	127.35	119.84
1	A	114	LEU	C-N-CA	6.01	127.35	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	308	LEU	N-CA-C	5.86	122.43	112.99
1	A	36	ASP	N-CA-C	5.86	120.72	112.93
1	A	125	LYS	N-CA-C	-5.81	98.42	110.80
1	D	36	ASP	N-CA-C	5.77	120.11	112.72
1	D	118	GLU	CA-CB-CG	5.76	125.63	114.10
3	F	308	LEU	N-CA-C	-5.74	103.87	112.54
3	C	300	SER	N-CA-C	-5.72	106.85	113.88
1	A	158	ILE	CA-C-N	5.68	125.69	119.89
1	A	158	ILE	C-N-CA	5.68	125.69	119.89
2	E	94	GLU	N-CA-C	5.67	118.67	111.69
3	C	247	THR	N-CA-C	5.66	117.59	110.24
1	D	3	ALA	N-CA-C	-5.61	105.72	113.18
3	C	309	LYS	CB-CG-CD	5.60	124.19	111.30
1	A	7	THR	N-CA-C	5.60	118.19	110.35
1	D	105	ALA	N-CA-C	5.55	117.28	108.79
2	E	153	SER	N-CA-C	5.54	118.50	109.24
3	C	308	LEU	CA-C-N	5.51	131.61	121.70
3	C	308	LEU	C-N-CA	5.51	131.61	121.70
3	C	309	LYS	CD-CE-NZ	5.51	129.52	111.90
3	F	19	ASN	CA-C-N	5.44	125.53	119.87
3	F	19	ASN	C-N-CA	5.44	125.53	119.87
2	E	213	ILE	CA-C-N	-5.43	114.08	122.49
2	E	213	ILE	C-N-CA	-5.43	114.08	122.49
1	A	129	GLN	N-CA-CB	-5.38	100.58	109.72
3	C	310	GLU	N-CA-C	-5.37	106.31	112.92
3	C	249	THR	N-CA-C	-5.33	105.11	111.03
1	D	158	ILE	CA-C-N	5.25	125.19	119.78
1	D	158	ILE	C-N-CA	5.25	125.19	119.78
2	B	342	LYS	N-CA-C	-5.23	102.53	110.28
3	C	141	ASN	N-CA-C	-5.22	106.49	112.92
3	C	65	ILE	N-CA-C	-5.22	98.48	109.34
3	C	305	ALA	N-CA-C	-5.22	105.49	111.07
2	E	103	LEU	N-CA-C	5.21	117.37	111.02
2	E	386	ILE	N-CA-C	5.20	115.41	110.42
3	F	337	THR	N-CA-C	5.18	116.74	108.41
1	A	105	ALA	N-CA-C	5.15	116.90	108.76
3	F	344	THR	N-CA-C	5.11	116.95	109.84
3	C	223	GLN	N-CA-C	-5.09	105.65	111.14
3	C	125	SER	N-CA-C	5.06	115.84	108.14
2	B	249	VAL	N-CA-C	5.06	115.28	110.42
3	C	212	LEU	N-CA-C	5.04	117.16	111.11
2	B	340	ASN	N-CA-C	5.04	117.16	107.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	228	ALA	CA-C-N	5.03	125.02	119.89
2	B	228	ALA	C-N-CA	5.03	125.02	119.89
3	F	184	TYR	CA-CB-CG	-5.00	104.89	113.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	308	LEU	Peptide
3	C	64	GLN	Peptide
1	D	118	GLU	Peptide
3	F	312	MET	Peptide
3	F	313	GLU	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	2544	0	2543	85	0
1	D	2544	0	2543	110	0
2	B	3289	0	3251	79	0
2	E	3281	0	3239	85	0
3	C	3537	0	3404	96	0
3	F	3516	0	3388	111	0
4	A	5	0	0	2	0
4	D	5	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	D	1	0	0	0	0
6	A	10	0	0	0	0
6	B	5	0	0	1	0
6	C	5	0	0	0	0
6	E	10	0	0	0	0
6	F	10	0	0	0	0
7	B	6	0	8	1	0
7	C	18	0	24	2	0
7	F	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	7	0	0	0	0
8	B	18	0	0	3	0
8	C	22	0	0	2	0
8	D	9	0	0	0	0
8	E	17	0	0	4	0
8	F	20	0	0	4	0
All	All	18888	0	18408	540	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 15.

All (540) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:ASN:HB2	2:B:366:LEU:HD11	1.34	1.06
1:A:126:ARG:O	1:A:128:GLU:N	1.96	0.98
3:F:160:SER:HB2	3:F:163:GLU:H	1.33	0.94
2:E:20:ASN:HB2	2:E:366:LEU:HD11	1.50	0.91
1:D:5:ASN:ND2	3:F:318:TYR:OH	2.05	0.89
1:A:129:GLN:CD	1:A:130:THR:H	1.81	0.88
3:F:100:LYS:HA	3:F:102:LEU:H	1.39	0.87
3:F:216:ARG:NH1	7:F:503:GOL:O2	2.08	0.86
2:B:324:TYR:OH	2:B:339:ARG:NH1	2.09	0.86
3:C:156:VAL:HG13	3:C:167:LEU:HD23	1.56	0.86
3:C:160:SER:HB2	3:C:163:GLU:H	1.40	0.85
1:D:172:GLN:HE22	1:D:282:VAL:HG23	1.44	0.82
1:A:203:ASP:OD2	1:A:241:ARG:NH2	2.12	0.82
1:A:269:LYS:NZ	1:A:299:GLU:OE1	2.13	0.82
3:C:337:THR:HA	3:C:366:THR:HB	1.60	0.81
3:F:100:LYS:HG2	3:F:101:TRP:HA	1.61	0.81
3:F:9:ASN:HB2	3:F:112:TYR:HB2	1.64	0.80
2:E:140:TYR:CE2	2:E:217:LYS:HG3	2.17	0.79
1:A:221:GLN:NE2	1:D:220:GLN:OE1	2.15	0.79
3:C:308:LEU:HB3	3:C:313:GLU:HB3	1.65	0.79
3:C:308:LEU:N	3:C:309:LYS:HB3	1.99	0.78
1:A:138:ALA:HA	1:A:141:LYS:HD2	1.66	0.77
3:F:242:ILE:HD12	3:F:422:ILE:HG12	1.67	0.77
2:E:41:LEU:HD22	2:E:285:VAL:HG21	1.67	0.76
3:C:308:LEU:H	3:C:309:LYS:HB3	1.48	0.76
3:F:216:ARG:HH12	7:F:503:GOL:HO2	1.34	0.75
2:B:39:GLU:HG2	2:B:339:ARG:HH21	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:140:TYR:CZ	2:E:217:LYS:HG3	2.23	0.74
3:F:254:MET:HE3	3:F:280:ARG:NH1	2.03	0.73
1:D:88:ASN:HB3	1:D:93:SER:OG	1.88	0.73
2:E:225:LYS:O	8:E:516:HOH:O	2.07	0.73
2:B:137:SER:HB3	2:B:220:LEU:HD21	1.71	0.73
1:D:218:ALA:O	1:D:223:TYR:HB2	1.89	0.72
1:D:118:GLU:HB2	1:D:121:LYS:HB3	1.71	0.71
2:E:243:ASP:OD2	2:E:245:ARG:NH1	2.23	0.71
2:E:80:LEU:HB2	2:E:88:ILE:HB	1.70	0.71
1:D:167:LEU:HD21	1:D:169:TYR:CZ	2.25	0.71
1:D:192:ASN:HD22	1:D:206:LEU:HD12	1.56	0.71
1:A:126:ARG:HG2	1:A:129:GLN:HG3	1.73	0.70
3:C:291:PRO:HA	3:C:316:ASN:HB2	1.73	0.69
1:D:224:LYS:HD2	1:D:251:ASP:OD2	1.92	0.69
2:E:68:ASP:HB2	2:E:81:VAL:HG13	1.75	0.69
2:B:2:GLU:OE2	8:B:503:HOH:O	2.12	0.68
3:F:267:ILE:HD11	3:F:292:TYR:CZ	2.28	0.68
3:F:156:VAL:HG13	3:F:167:LEU:HD23	1.74	0.68
3:C:261:LEU:HD22	3:C:333:ASN:HB3	1.76	0.67
1:A:86:ALA:HA	1:A:97:MET:HE1	1.77	0.67
3:C:116:ILE:HG21	3:C:168:LEU:HD22	1.76	0.67
3:C:344:THR:HG22	3:C:347:ALA:H	1.59	0.67
3:F:283:ARG:HH11	3:F:283:ARG:CG	2.08	0.66
2:B:1:MET:HE3	2:B:7:ILE:HG12	1.78	0.66
2:E:93:GLN:O	2:E:97:LEU:HG	1.96	0.65
3:F:106:ARG:NH1	8:F:612:HOH:O	2.28	0.65
1:D:226:ILE:HG21	1:D:276:ILE:HD11	1.79	0.65
2:E:139:TYR:CD2	3:F:65:ILE:HG22	2.32	0.65
1:A:187:THR:OG1	1:A:288:ASP:HB3	1.97	0.64
1:A:21:GLY:HA2	1:A:126:ARG:HH21	1.63	0.64
1:D:194:ARG:NH1	1:D:205:ASP:OD2	2.30	0.64
1:D:295:MET:HE1	1:D:300:LEU:HD12	1.78	0.64
3:F:340:ILE:HD11	3:F:367:THR:HB	1.80	0.64
1:D:72:VAL:HG13	1:D:82:VAL:HG11	1.79	0.64
3:C:253:ARG:HD3	3:C:366:THR:HG21	1.79	0.64
2:E:181:LYS:NZ	2:E:185:ASP:OD2	2.31	0.63
3:F:267:ILE:HD11	3:F:292:TYR:CE2	2.32	0.63
3:F:309:LYS:NZ	3:F:314:ALA:HB2	2.13	0.63
2:B:41:LEU:HD22	2:B:285:VAL:HG21	1.81	0.63
3:C:129:SER:HA	7:C:503:GOL:H11	1.81	0.63
3:F:240:LEU:HB3	3:F:242:ILE:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:OD1	1:A:231:ARG:NE	2.31	0.63
1:D:119:LEU:HB3	1:D:139:ILE:HD11	1.81	0.63
1:D:192:ASN:HD22	1:D:206:LEU:CD1	2.12	0.62
1:D:79:ARG:HD2	3:F:311:ARG:HE	1.64	0.62
3:C:310:GLU:HG2	3:C:312:MET:HB2	1.81	0.62
1:D:135:PRO:C	1:D:137:SER:H	2.06	0.62
1:D:98:VAL:HG13	1:D:107:ILE:HD12	1.81	0.61
1:A:117:GLU:HA	1:A:120:VAL:HG22	1.81	0.61
1:A:217:MET:HE1	1:D:218:ALA:HA	1.82	0.61
1:D:86:ALA:HA	1:D:97:MET:HE1	1.82	0.61
1:A:141:LYS:O	1:A:145:GLN:HB2	1.99	0.61
3:C:188:ASP:OD1	3:C:189:ASP:N	2.33	0.61
1:A:6:ASN:HB3	1:D:261:TYR:CE1	2.36	0.61
2:E:63:MET:HG2	2:E:124:TRP:CD1	2.36	0.61
2:B:1:MET:HE2	2:B:10:ARG:HH11	1.64	0.60
3:F:186:TYR:HD1	3:F:188:ASP:H	1.47	0.60
3:F:214:ILE:HA	3:F:218:ILE:HD13	1.83	0.60
2:B:68:ASP:HB2	2:B:81:VAL:HG23	1.82	0.60
2:E:240:VAL:HG22	2:E:246:GLU:HG2	1.82	0.60
3:F:104:ARG:HG3	3:F:108:GLU:CD	2.26	0.60
3:F:59:PRO:HG2	3:F:184:TYR:HB3	1.83	0.60
2:B:179:SER:O	2:B:181:LYS:N	2.33	0.60
1:A:218:ALA:O	1:A:223:TYR:HB2	2.01	0.60
1:A:24:LYS:HB2	4:A:401:PO4:O1	2.01	0.60
1:A:237:GLU:O	1:A:241:ARG:HD3	2.01	0.59
2:E:61:LYS:HB2	2:E:297:VAL:HG23	1.84	0.59
1:D:235:TYR:C	1:D:238:PRO:HD2	2.27	0.59
2:E:148:GLU:HG2	8:E:515:HOH:O	2.02	0.59
1:A:194:ARG:NH1	1:A:205:ASP:OD2	2.36	0.59
1:D:16:LEU:HB2	1:D:85:ASP:HA	1.85	0.59
2:E:113:GLU:HG3	2:E:242:THR:HG22	1.85	0.59
2:E:232:LYS:HE3	2:E:259:ASN:HD21	1.67	0.59
1:A:129:GLN:NE2	1:A:130:THR:OG1	2.36	0.59
1:D:52:GLY:HA3	1:D:56:MET:HE3	1.84	0.59
1:D:172:GLN:NE2	1:D:282:VAL:HG23	2.14	0.59
1:D:256:ARG:HG3	1:D:267:ILE:HD13	1.84	0.59
3:C:59:PRO:HG2	3:C:184:TYR:HB3	1.85	0.59
2:E:39:GLU:HG2	2:E:339:ARG:HH12	1.68	0.58
1:A:167:LEU:HB3	1:D:190:LEU:HD21	1.85	0.58
3:C:327:GLU:O	3:C:329:LYS:HG2	2.02	0.58
2:E:23:SER:HB3	2:E:66:TYR:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ALA:O	1:D:22:SER:OG	2.19	0.58
3:C:271:GLY:HA3	3:C:339:VAL:HG11	1.84	0.58
1:D:130:THR:OG1	1:D:132:LYS:NZ	2.18	0.58
2:E:290:GLN:HG3	2:E:291:SER:N	2.19	0.58
3:F:144:ILE:HD12	3:F:152:LEU:HD13	1.85	0.58
1:A:52:GLY:HA3	1:A:56:MET:HE3	1.85	0.57
1:A:120:VAL:HG11	1:A:136:LYS:HD3	1.85	0.57
1:A:277:GLN:HG3	1:A:278:GLY:N	2.19	0.57
3:C:9:ASN:HB2	3:C:112:TYR:HB2	1.85	0.57
3:F:283:ARG:HH11	3:F:283:ARG:HG2	1.69	0.57
1:D:145:GLN:O	1:D:149:THR:HG23	2.03	0.57
3:F:341:GLU:HA	3:F:391:PHE:CE2	2.39	0.57
3:C:105:THR:O	3:C:109:VAL:HG23	2.04	0.57
1:D:8:HIS:C	1:D:9:HIS:HD2	2.12	0.57
3:F:413:VAL:HG22	3:F:433:ILE:HG12	1.86	0.57
3:C:129:SER:OG	3:C:130:LYS:N	2.38	0.57
1:D:136:LYS:HA	1:D:139:ILE:HG22	1.85	0.57
2:B:41:LEU:HD12	2:B:298:ILE:HD11	1.85	0.57
1:A:135:PRO:HG2	1:A:138:ALA:H	1.69	0.57
2:B:162:ILE:HD12	3:C:23:ASP:HB3	1.87	0.57
1:D:118:GLU:HA	1:D:121:LYS:H	1.68	0.57
3:F:52:ASP:OD1	3:F:53:THR:N	2.38	0.57
1:A:146:LEU:HD21	1:A:150:LYS:HD2	1.87	0.57
3:F:254:MET:HE3	3:F:280:ARG:HH12	1.67	0.57
1:A:129:GLN:HG2	1:A:130:THR:HG23	1.86	0.56
1:D:90:SER:C	1:D:149:THR:HG21	2.29	0.56
1:A:184:LEU:HD11	1:A:227:LEU:HD23	1.87	0.56
2:B:39:GLU:CG	2:B:339:ARG:HH21	2.18	0.56
3:C:268:LEU:HD23	3:C:334:ILE:HD12	1.86	0.56
1:D:154:ASP:OD1	1:D:156:LYS:HG2	2.04	0.56
2:E:124:TRP:CD1	2:E:124:TRP:H	2.22	0.56
3:F:62:SER:HB3	3:F:184:TYR:CD2	2.40	0.56
3:C:147:ILE:HG13	3:C:152:LEU:HA	1.86	0.56
1:D:91:LEU:HB2	1:D:149:THR:CG2	2.36	0.56
3:F:114:CYS:SG	3:F:161:VAL:HG22	2.46	0.56
2:E:93:GLN:NE2	8:E:514:HOH:O	2.18	0.56
3:F:188:ASP:OD1	3:F:189:ASP:N	2.38	0.56
3:F:312:MET:O	3:F:313:GLU:HG2	2.06	0.56
1:A:195:ASP:HB3	1:A:198:ASN:HB3	1.88	0.56
1:D:254:LEU:HB3	1:D:271:LEU:HD22	1.88	0.56
1:A:88:ASN:CG	1:A:89:SER:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:TYR:OH	2:B:217:LYS:HD3	2.06	0.55
3:C:99:ILE:HD12	3:C:109:VAL:HG21	1.86	0.55
1:D:114:LEU:HB2	1:D:115:PRO:HD2	1.88	0.55
2:E:62:TYR:HB3	2:E:122:MET:HE1	1.87	0.55
3:F:267:ILE:HD13	3:F:335:ILE:HD12	1.88	0.55
3:C:364:ILE:HG12	3:C:432:VAL:HG22	1.88	0.55
2:E:112:VAL:HG11	2:E:115:ARG:CZ	2.36	0.55
1:D:25:SER:OG	1:D:26:THR:N	2.40	0.55
1:A:114:LEU:HD11	1:A:122:ARG:NH2	2.21	0.55
3:C:313:GLU:CD	3:C:315:ASP:HA	2.32	0.55
2:E:162:ILE:HD13	3:F:23:ASP:HB3	1.87	0.55
2:E:236:ILE:HD11	2:E:258:ILE:HD12	1.87	0.55
2:E:369:GLU:HG2	2:E:371:TYR:HE2	1.71	0.55
3:F:105:THR:O	3:F:109:VAL:HG23	2.06	0.55
1:D:269:LYS:NZ	1:D:299:GLU:OE1	2.40	0.54
3:C:307:LEU:HA	3:C:309:LYS:HG2	1.88	0.54
1:D:16:LEU:HD22	1:D:112:PHE:HE1	1.72	0.54
1:D:94:LEU:HD21	1:D:155:PHE:HE1	1.72	0.54
3:F:187:ILE:HG22	3:F:187:ILE:O	2.07	0.54
3:C:371:LEU:HG	3:C:395:PRO:HD2	1.88	0.54
1:D:181:ILE:HD11	1:D:276:ILE:HD13	1.89	0.54
1:D:219:LYS:HZ1	1:D:249:ASP:C	2.16	0.54
3:C:118:VAL:HB	3:C:154:LEU:HB3	1.89	0.54
1:D:290:ASN:HB2	1:D:311:ASP:H	1.73	0.54
2:E:121:LEU:HD23	2:E:127:LEU:HD22	1.90	0.54
3:C:299:LYS:HG3	3:C:302:GLY:HA3	1.90	0.54
3:C:313:GLU:O	3:C:315:ASP:HB3	2.08	0.54
1:D:22:SER:HA	1:D:114:LEU:HD11	1.90	0.54
2:E:302:THR:HB	2:E:305:LEU:HD11	1.90	0.54
3:F:13:LEU:HD21	3:F:40:ALA:HB1	1.89	0.54
2:B:74:ARG:HG2	2:B:76:GLU:HG2	1.89	0.54
1:D:207:LEU:HD11	1:D:212:ALA:HB2	1.90	0.54
2:E:237:LEU:HD13	2:E:359:LEU:HD11	1.90	0.53
3:F:147:ILE:HG13	3:F:152:LEU:HA	1.89	0.53
2:E:251:ASP:OD1	2:E:253:LEU:HB2	2.08	0.53
1:A:91:LEU:H	1:A:149:THR:HG21	1.73	0.53
2:B:68:ASP:HB2	2:B:81:VAL:CG2	2.38	0.53
2:E:147:ALA:O	2:E:151:VAL:HG22	2.08	0.53
1:A:22:SER:HA	1:A:114:LEU:HD12	1.90	0.53
3:C:308:LEU:O	3:C:313:GLU:HB3	2.08	0.53
1:D:128:GLU:N	1:D:128:GLU:OE1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:238:LYS:NZ	2:E:359:LEU:O	2.30	0.53
1:D:79:ARG:HD2	3:F:311:ARG:NE	2.23	0.53
3:F:337:THR:HA	3:F:366:THR:HB	1.91	0.53
3:F:62:SER:HB3	3:F:184:TYR:HD2	1.74	0.53
1:D:126:ARG:HD2	1:D:132:LYS:NZ	2.24	0.53
2:B:361:ILE:HD11	2:B:372:GLU:HG2	1.91	0.52
2:E:323:VAL:O	3:F:65:ILE:HD11	2.09	0.52
2:B:204:LEU:HD21	8:C:609:HOH:O	2.09	0.52
3:F:313:GLU:C	3:F:315:ASP:HB2	2.35	0.52
1:A:91:LEU:O	1:A:95:GLN:HG3	2.09	0.52
3:C:125:SER:OG	3:C:126:THR:N	2.39	0.52
1:D:88:ASN:OD1	1:D:90:SER:HB3	2.10	0.52
3:F:1:MET:HE1	3:F:118:VAL:HG13	1.91	0.52
1:A:207:LEU:HD11	1:A:212:ALA:HB2	1.92	0.52
1:A:232:GLU:HG2	1:A:258:THR:HA	1.92	0.52
3:C:129:SER:C	3:C:130:LYS:HD3	2.35	0.51
2:B:91:LEU:HD23	2:B:92:ASP:N	2.26	0.51
1:A:11:PRO:HG3	1:A:79:ARG:HA	1.92	0.51
1:A:267:ILE:HD12	1:A:271:LEU:HD12	1.92	0.51
2:B:115:ARG:HG2	2:B:239:GLU:HG2	1.92	0.51
3:C:55:TYR:CZ	3:C:60:GLU:HG3	2.46	0.51
3:C:344:THR:HG22	3:C:346:GLU:N	2.26	0.51
1:D:91:LEU:HB2	1:D:149:THR:HG22	1.91	0.51
2:E:43:GLU:OE2	8:E:509:HOH:O	2.18	0.51
3:F:394:THR:HG23	3:F:397:GLU:OE1	2.10	0.51
1:A:31:PHE:CE1	1:A:35:GLU:HG3	2.46	0.51
1:A:140:GLU:O	1:A:140:GLU:HG3	2.10	0.51
1:D:160:ARG:HH22	1:D:162:LEU:HD22	1.76	0.51
1:D:22:SER:HB2	1:D:112:PHE:HB3	1.93	0.51
1:D:135:PRO:C	1:D:137:SER:N	2.69	0.51
3:F:129:SER:OG	3:F:130:LYS:N	2.41	0.51
1:D:125:LYS:O	1:D:125:LYS:HG3	2.11	0.51
1:A:145:GLN:O	1:A:149:THR:HG23	2.11	0.51
1:A:228:LEU:HD22	1:A:268:LYS:HG2	1.93	0.51
2:B:91:LEU:HD22	2:B:96:CYS:SG	2.51	0.51
1:D:116:VAL:O	1:D:120:VAL:HG23	2.10	0.51
1:A:226:ILE:HD11	1:A:280:TYR:CZ	2.46	0.51
1:A:256:ARG:HG3	1:A:267:ILE:HD13	1.93	0.51
2:B:84:ASN:HB2	2:B:86:TYR:CD2	2.46	0.51
2:B:277:LYS:NZ	8:B:510:HOH:O	2.42	0.51
1:D:90:SER:HA	1:D:145:GLN:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:VAL:HG13	2:B:199:ARG:HD3	1.93	0.51
3:C:338:GLU:HG2	3:C:366:THR:HG22	1.92	0.51
3:F:266:PRO:HB3	3:F:290:HIS:HB3	1.93	0.51
2:B:236:ILE:HD12	2:B:254:SER:HB2	1.92	0.50
2:B:237:LEU:HD13	2:B:359:LEU:HD11	1.91	0.50
1:D:294:ASP:OD1	1:D:298:ARG:NH1	2.35	0.50
3:F:291:PRO:HA	3:F:316:ASN:HB2	1.92	0.50
3:C:1:MET:HE3	3:C:2:ILE:H	1.77	0.50
3:F:283:ARG:CG	3:F:283:ARG:NH1	2.70	0.50
2:B:156:TYR:O	2:B:160:GLN:HG3	2.12	0.50
3:C:33:ASN:O	3:C:53:THR:OG1	2.21	0.50
2:E:188:PRO:HG2	2:E:191:ILE:HG12	1.92	0.50
2:B:154:SER:HB2	3:C:39:ASN:HD21	1.77	0.50
2:E:136:PHE:HE1	2:E:220:LEU:HD11	1.77	0.50
3:F:100:LYS:HA	3:F:102:LEU:N	2.18	0.50
2:E:266:TYR:HE2	2:E:277:LYS:HD3	1.76	0.50
2:B:11:ILE:HG12	2:B:377:VAL:HG11	1.93	0.50
2:E:262:ASP:OD1	2:E:263:PHE:N	2.45	0.50
3:F:1:MET:HE3	3:F:1:MET:HA	1.94	0.50
3:F:399:GLN:HG2	3:F:415:TYR:CE2	2.47	0.49
3:C:134:MET:HE1	3:C:377:PHE:HB2	1.93	0.49
2:E:103:LEU:HD11	2:E:258:ILE:HD11	1.95	0.49
2:B:253:LEU:HD11	2:B:265:HIS:CE1	2.47	0.49
2:E:103:LEU:HA	2:E:106:ARG:HD2	1.94	0.49
2:E:372:GLU:O	2:E:376:LEU:HD23	2.12	0.49
1:A:10:PHE:C	3:C:311:ARG:HH21	2.20	0.49
3:C:4:GLN:HE21	3:C:47:ASP:CG	2.21	0.49
1:D:236:ARG:O	1:D:240:GLU:HG2	2.12	0.49
1:A:98:VAL:O	1:A:102:THR:HB	2.13	0.49
2:B:201:PHE:HA	3:C:35:GLN:HG3	1.93	0.49
3:C:275:LEU:HA	8:C:619:HOH:O	2.12	0.49
2:B:150:LEU:HD13	2:B:156:TYR:CE2	2.47	0.49
3:F:116:ILE:HG21	3:F:168:LEU:HD22	1.94	0.49
3:F:283:ARG:NH2	8:F:605:HOH:O	2.45	0.49
1:A:224:LYS:HD2	1:A:251:ASP:CG	2.37	0.49
1:D:287:ASP:OD1	1:D:288:ASP:N	2.39	0.49
2:E:60:LYS:HE3	2:E:62:TYR:OH	2.13	0.49
2:E:369:GLU:HG2	2:E:371:TYR:CE2	2.48	0.49
2:B:16:LYS:HE3	2:B:368:GLU:OE1	2.13	0.49
2:B:259:ASN:OD1	2:B:261:ASP:HB2	2.12	0.49
2:E:14:PHE:CD2	2:E:377:VAL:HG21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:LEU:HD12	2:E:298:ILE:HD11	1.95	0.49
2:B:33:VAL:N	6:B:403:SO4:O2	2.47	0.48
1:A:129:GLN:CG	1:A:130:THR:H	2.26	0.48
1:D:219:LYS:HE2	1:D:225:VAL:HG23	1.95	0.48
3:F:327:GLU:O	3:F:329:LYS:HG2	2.13	0.48
2:B:180:ALA:HA	2:B:183:LEU:HG	1.94	0.48
2:E:319:TYR:HA	2:E:322:LEU:HD12	1.96	0.48
3:F:105:THR:OG1	3:F:108:GLU:OE1	2.20	0.48
1:D:138:ALA:HA	1:D:141:LYS:HZ3	1.78	0.48
1:D:143:VAL:O	1:D:147:GLN:HG2	2.13	0.48
2:E:38:ILE:HG12	2:E:339:ARG:CZ	2.43	0.48
1:D:178:LYS:HE3	1:D:222:GLY:HA3	1.96	0.48
1:D:121:LYS:O	1:D:121:LYS:HG3	2.13	0.48
1:D:297:ARG:O	1:D:301:ALA:HA	2.14	0.48
2:E:133:ASN:ND2	2:E:135:GLU:HB2	2.28	0.48
3:F:133:PHE:HB2	3:F:144:ILE:HG13	1.96	0.48
3:C:360:PHE:O	3:C:435:ARG:HD2	2.14	0.48
3:F:263:MET:HE3	3:F:286:TYR:CD1	2.49	0.48
3:F:309:LYS:HZ3	3:F:314:ALA:HB2	1.78	0.48
3:C:306:ALA:O	3:C:309:LYS:HE2	2.14	0.47
3:C:323:TRP:CZ3	3:C:358:LEU:HD11	2.48	0.47
1:D:11:PRO:HG3	1:D:79:ARG:HA	1.97	0.47
2:E:88:ILE:HD12	2:E:127:LEU:HD11	1.95	0.47
2:B:5:THR:HA	2:B:8:LYS:HE2	1.96	0.47
3:F:127:TRP:CE3	3:F:178:THR:HG21	2.49	0.47
3:C:359:ASN:HA	3:C:435:ARG:HH12	1.79	0.47
2:E:174:ASP:OD2	2:E:186:LYS:HE2	2.13	0.47
2:E:332:LEU:O	2:E:336:ILE:HG13	2.13	0.47
1:D:79:ARG:HD2	3:F:311:ARG:CD	2.45	0.47
1:D:285:LEU:HD22	1:D:296:TRP:CD2	2.50	0.47
2:E:166:PRO:HA	2:E:169:LEU:HB2	1.96	0.47
1:A:207:LEU:HD22	1:A:246:TYR:HD2	1.79	0.47
2:B:73:ARG:HA	2:B:109:TRP:CE3	2.49	0.47
2:B:304:PHE:CD2	2:B:356:ALA:HB2	2.50	0.47
3:C:97:GLN:NE2	3:C:106:ARG:HH11	2.12	0.47
2:E:81:VAL:HA	2:E:86:TYR:O	2.15	0.47
2:B:310:PRO:HB3	2:B:352:TRP:CD2	2.49	0.47
1:D:146:LEU:O	1:D:150:LYS:N	2.43	0.47
2:E:294:GLU:HG2	2:E:319:TYR:CZ	2.48	0.47
2:B:209:TYR:O	2:B:213:ILE:HG13	2.15	0.47
1:D:270:GLU:O	1:D:274:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:272:CYS:SG	3:F:294:ALA:HB1	2.55	0.47
1:A:286:LEU:HD23	1:A:305:PHE:HB2	1.96	0.47
3:F:1:MET:CE	3:F:118:VAL:HG13	2.45	0.46
3:C:218:ILE:HG21	3:C:224:PHE:HB2	1.97	0.46
1:D:8:HIS:C	1:D:9:HIS:CD2	2.93	0.46
3:F:310:GLU:HG2	3:F:312:MET:HB2	1.97	0.46
3:F:113:PRO:HA	3:F:159:LYS:O	2.16	0.46
1:A:146:LEU:O	1:A:150:LYS:N	2.47	0.46
1:A:263:LYS:HB3	1:A:263:LYS:HE2	1.75	0.46
3:C:1:MET:HE3	3:C:1:MET:HA	1.98	0.46
3:C:399:GLN:HG2	3:C:415:TYR:CE2	2.51	0.46
1:D:91:LEU:O	1:D:95:GLN:HG3	2.14	0.46
3:F:170:PHE:HD2	3:F:171:ILE:HD13	1.80	0.46
1:A:217:MET:CE	1:D:218:ALA:HA	2.45	0.46
3:C:57:TYR:CZ	3:C:75:VAL:HG22	2.50	0.46
2:B:350:ASN:HB3	8:B:516:HOH:O	2.16	0.46
3:F:184:TYR:O	3:F:185:THR:OG1	2.34	0.46
1:A:98:VAL:HG13	1:A:107:ILE:HD12	1.97	0.46
2:B:66:TYR:CD2	7:B:404:GOL:H31	2.51	0.46
1:D:257:ASP:O	1:D:260:ASP:HB2	2.16	0.46
2:E:124:TRP:CH2	2:E:223:PHE:HB2	2.51	0.46
2:B:92:ASP:OD2	2:B:95:GLN:HB2	2.16	0.45
1:D:290:ASN:H	1:D:310:GLY:HA3	1.80	0.45
3:F:263:MET:HE3	3:F:286:TYR:CG	2.51	0.45
1:A:173:ASP:HB3	1:A:176:LEU:HD12	1.98	0.45
2:E:122:MET:HB2	2:E:230:PHE:CD2	2.51	0.45
1:A:290:ASN:HB2	1:A:311:ASP:H	1.81	0.45
2:B:53:VAL:HG11	2:B:300:PRO:HB3	1.99	0.45
3:C:86:GLU:CD	3:C:86:GLU:H	2.24	0.45
3:C:88:LEU:O	3:C:197:ARG:NH2	2.31	0.45
2:B:248:PHE:CD1	2:B:250:ASN:HB2	2.51	0.45
3:C:187:ILE:O	3:C:219:LYS:HE3	2.16	0.45
1:D:240:GLU:HA	1:D:243:LEU:HB2	1.99	0.45
2:E:320:LEU:HA	2:E:323:VAL:HG22	1.97	0.45
3:F:170:PHE:O	3:F:174:THR:HG23	2.17	0.45
2:E:11:ILE:HG12	2:E:377:VAL:CG1	2.47	0.45
2:B:11:ILE:HG12	2:B:377:VAL:CG1	2.47	0.45
2:B:151:VAL:HG12	2:B:206:LEU:HD13	1.99	0.45
2:E:150:LEU:HD13	2:E:156:TYR:CE1	2.52	0.45
3:C:52:ASP:OD1	3:C:53:THR:N	2.50	0.45
2:E:384:GLU:HA	2:E:387:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:282:MET:HE1	3:F:316:ASN:HD21	1.81	0.45
3:F:361:HIS:HD2	3:F:362:LYS:HG3	1.82	0.45
2:B:22:PHE:N	2:B:355:ASN:OD1	2.47	0.45
3:C:80:CYS:HB3	3:C:88:LEU:HD21	1.99	0.45
1:D:79:ARG:HD2	3:F:311:ARG:HD2	1.98	0.45
1:D:137:SER:O	1:D:140:GLU:HB3	2.16	0.45
3:F:15:LEU:HA	3:F:106:ARG:NH2	2.31	0.45
3:F:16:LEU:O	3:F:18:LYS:HE2	2.18	0.45
3:C:126:THR:HB	7:C:502:GOL:O2	2.18	0.44
3:C:310:GLU:CG	3:C:312:MET:HB2	2.45	0.44
3:F:402:ILE:O	3:F:406:VAL:HG22	2.16	0.44
1:A:207:LEU:HD22	1:A:246:TYR:CD2	2.51	0.44
2:B:327:ASP:OD1	2:B:327:ASP:N	2.43	0.44
3:C:272:CYS:SG	3:C:294:ALA:HB1	2.57	0.44
3:C:306:ALA:O	3:C:309:LYS:HG2	2.18	0.44
1:D:262:ARG:HH22	1:D:270:GLU:CD	2.25	0.44
1:A:22:SER:HB2	1:A:112:PHE:HB3	2.00	0.44
1:A:114:LEU:HD23	1:A:115:PRO:HD2	2.00	0.44
1:A:215:LEU:HD22	1:A:225:VAL:HG13	1.98	0.44
3:C:185:THR:O	3:C:186:TYR:HB3	2.18	0.44
3:C:302:GLY:HA2	3:C:319:PHE:CE1	2.53	0.44
1:D:118:GLU:HA	1:D:121:LYS:HB3	2.00	0.44
2:E:253:LEU:HA	2:E:253:LEU:HD23	1.62	0.44
2:B:292:ASP:HB2	2:B:293:GLU:HG3	2.00	0.44
3:C:36:LEU:O	3:C:37:ILE:HD13	2.18	0.44
3:C:114:CYS:SG	3:C:161:VAL:HG22	2.57	0.44
2:E:169:LEU:HD23	2:E:169:LEU:HA	1.68	0.44
3:C:2:ILE:HG12	3:C:49:VAL:HG22	1.99	0.44
3:C:77:LEU:HD23	3:C:77:LEU:HA	1.70	0.44
1:D:277:GLN:O	1:D:279:LYS:HG2	2.18	0.44
1:D:308:ASN:CG	1:D:309:TYR:H	2.25	0.44
2:E:55:GLU:CD	2:E:301:ARG:HG2	2.42	0.44
1:A:146:LEU:CD2	1:A:150:LYS:HD2	2.48	0.44
2:E:139:TYR:CE2	3:F:65:ILE:HG22	2.52	0.44
3:C:304:TYR:O	3:C:308:LEU:HD12	2.18	0.43
1:D:126:ARG:CD	1:D:132:LYS:HZ3	2.31	0.43
1:D:148:TYR:O	1:D:151:GLU:HB3	2.18	0.43
3:F:242:ILE:CD1	3:F:422:ILE:HG23	2.48	0.43
3:C:101:TRP:HA	3:C:101:TRP:CE3	2.53	0.43
2:E:118:GLN:HG3	2:E:237:LEU:HG	2.00	0.43
3:F:280:ARG:HD3	8:F:605:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:309:LYS:HZ2	3:F:314:ALA:HB2	1.83	0.43
1:A:209:THR:N	1:A:210:PRO:HD2	2.33	0.43
3:C:113:PRO:HA	3:C:159:LYS:O	2.18	0.43
3:C:142:ILE:HD13	3:C:142:ILE:HA	1.81	0.43
1:D:2:SER:OG	3:F:327:GLU:OE1	2.36	0.43
2:E:117:ILE:HD13	2:E:258:ILE:HD11	1.99	0.43
3:F:137:ARG:HB2	3:F:138:TYR:CD1	2.53	0.43
3:F:144:ILE:HG22	3:F:146:PRO:HD3	2.00	0.43
1:A:126:ARG:C	1:A:128:GLU:H	2.05	0.43
2:E:91:LEU:HB3	2:E:96:CYS:SG	2.59	0.43
1:A:242:PHE:CD1	1:A:242:PHE:C	2.96	0.43
1:D:135:PRO:HD2	1:D:138:ALA:HB3	1.99	0.43
3:F:218:ILE:HG21	3:F:224:PHE:HB2	2.01	0.43
2:B:25:THR:OG1	2:B:387:GLU:OE2	2.19	0.43
2:B:168:TYR:O	2:B:172:VAL:HG23	2.18	0.43
3:C:170:PHE:O	3:C:174:THR:HG23	2.19	0.43
1:D:178:LYS:HB2	1:D:223:TYR:CE1	2.54	0.43
2:E:243:ASP:OD1	2:E:243:ASP:N	2.50	0.43
1:D:240:GLU:OE1	1:D:250:TYR:OH	2.35	0.43
2:E:253:LEU:HD11	2:E:265:HIS:HD2	1.83	0.43
1:D:123:CYS:HB3	1:D:134:ILE:CG2	2.48	0.43
3:F:188:ASP:OD1	3:F:190:HIS:N	2.38	0.43
3:F:402:ILE:HG13	3:F:431:VAL:HG11	2.01	0.43
1:A:86:ALA:HA	1:A:97:MET:CE	2.48	0.43
2:B:91:LEU:CD2	2:B:96:CYS:SG	3.07	0.43
1:D:90:SER:OG	1:D:91:LEU:N	2.48	0.43
2:E:121:LEU:HD23	2:E:127:LEU:HB2	2.00	0.43
2:E:139:TYR:HB2	3:F:67:PHE:HD2	1.83	0.43
3:F:3:LEU:CD1	3:F:118:VAL:HG22	2.48	0.43
3:F:304:TYR:O	3:F:308:LEU:HD12	2.19	0.43
3:F:104:ARG:HD2	3:F:104:ARG:HA	1.54	0.43
2:B:268:PHE:O	2:B:270:ASP:N	2.48	0.42
3:C:50:PHE:CE2	3:C:52:ASP:HB2	2.54	0.42
3:C:415:TYR:CE2	3:C:431:VAL:HG22	2.53	0.42
3:F:142:ILE:HG23	3:F:154:LEU:HD11	2.01	0.42
1:A:71:SER:HB3	1:D:67:MET:HE3	2.02	0.42
2:B:159:LEU:HD22	2:B:198:ILE:HG23	1.99	0.42
3:C:399:GLN:HG2	3:C:415:TYR:CZ	2.54	0.42
3:F:261:LEU:HD22	3:F:333:ASN:HB3	2.01	0.42
2:B:127:LEU:HD12	2:B:127:LEU:HA	1.57	0.42
2:B:232:LYS:NZ	2:B:261:ASP:OD2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:ARG:C	3:C:34:GLY:HA3	2.43	0.42
1:A:184:LEU:HD23	1:A:231:ARG:NH2	2.35	0.42
1:A:236:ARG:O	1:A:240:GLU:HG2	2.19	0.42
2:E:137:SER:HB3	2:E:220:LEU:HD21	2.01	0.42
1:A:24:LYS:HE3	4:A:401:PO4:O1	2.20	0.42
2:B:178:LEU:HB2	2:B:183:LEU:HD23	2.02	0.42
3:C:344:THR:O	3:C:348:ALA:N	2.52	0.42
2:E:256:GLN:HB3	2:E:263:PHE:CZ	2.54	0.42
2:E:266:TYR:CE2	2:E:277:LYS:HD3	2.55	0.42
2:B:243:ASP:HB2	2:B:245:ARG:H	1.83	0.42
3:C:83:PHE:HB3	3:C:84:PHE:CE1	2.55	0.42
3:F:142:ILE:HD11	3:F:171:ILE:HD11	2.00	0.42
1:A:120:VAL:HG12	1:A:139:ILE:HD12	2.02	0.42
2:B:101:GLN:O	2:B:102:GLY:C	2.62	0.42
1:D:8:HIS:CD2	1:D:8:HIS:N	2.88	0.42
1:D:295:MET:HE3	1:D:296:TRP:CE3	2.54	0.42
2:B:54:LYS:HB3	2:B:268:PHE:HB2	2.01	0.42
3:C:185:THR:HG22	3:C:186:TYR:N	2.35	0.42
3:F:55:TYR:CZ	3:F:60:GLU:HG3	2.55	0.42
2:B:90:HIS:O	2:B:91:LEU:HB3	2.20	0.42
3:C:62:SER:HB3	3:C:184:TYR:CD2	2.54	0.42
1:D:46:PHE:HE1	1:D:67:MET:HE2	1.85	0.42
1:D:243:LEU:HD13	1:D:250:TYR:CE2	2.55	0.42
3:F:283:ARG:NH1	3:F:283:ARG:HG3	2.34	0.42
3:F:334:ILE:HB	3:F:363:MET:HG3	2.02	0.42
1:A:137:SER:OG	1:A:138:ALA:N	2.52	0.41
1:D:235:TYR:O	1:D:238:PRO:HD2	2.19	0.41
2:B:74:ARG:O	2:B:77:ASP:HB2	2.19	0.41
1:D:195:ASP:HB3	1:D:198:ASN:HB3	2.02	0.41
3:F:275:LEU:HB3	3:F:278:TYR:HB3	2.01	0.41
3:F:313:GLU:HB3	3:F:315:ASP:OD2	2.20	0.41
2:B:246:GLU:OE1	2:B:362:PRO:HA	2.21	0.41
3:C:220:SER:HG	3:C:223:GLN:H	1.64	0.41
2:E:90:HIS:HE1	2:E:127:LEU:HD12	1.85	0.41
2:B:246:GLU:OE2	2:B:363:TYR:N	2.39	0.41
2:B:345:LEU:HD12	2:B:345:LEU:O	2.20	0.41
2:E:253:LEU:HD11	2:E:265:HIS:CD2	2.55	0.41
3:F:317:LEU:HA	3:F:317:LEU:HD12	1.76	0.41
2:B:23:SER:HB3	2:B:66:TYR:CE1	2.55	0.41
3:C:5:ILE:O	3:C:45:GLN:HA	2.21	0.41
1:D:16:LEU:HB3	1:D:24:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:LYS:O	2:E:267:GLN:HA	2.21	0.41
3:F:121:LEU:HD23	3:F:152:LEU:HD11	2.01	0.41
3:F:195:TYR:O	3:F:198:ILE:HG13	2.21	0.41
1:A:303:PRO:HB3	1:D:210:PRO:HG3	2.03	0.41
2:B:163:GLN:HA	2:B:168:TYR:CE1	2.56	0.41
2:B:391:ASP:HB3	2:B:394:LEU:HG	2.03	0.41
3:C:101:TRP:O	3:C:102:LEU:HD23	2.21	0.41
3:C:283:ARG:HB2	3:C:286:TYR:CD2	2.56	0.41
3:F:174:THR:O	3:F:178:THR:HG23	2.20	0.41
1:A:12:LYS:HE2	1:A:12:LYS:HB3	1.87	0.41
1:A:31:PHE:CZ	1:A:35:GLU:HG3	2.55	0.41
1:A:219:LYS:HE3	1:A:219:LYS:HB2	1.93	0.41
1:A:305:PHE:CE1	1:D:307:VAL:HG13	2.56	0.41
1:D:157:PRO:O	1:D:158:ILE:HD13	2.21	0.41
1:D:179:ALA:O	1:D:282:VAL:HA	2.21	0.41
2:E:136:PHE:CE1	2:E:220:LEU:HD11	2.53	0.41
3:F:154:LEU:HD12	3:F:155:ARG:H	1.86	0.41
1:A:270:GLU:O	1:A:274:GLU:HG3	2.21	0.41
1:D:178:LYS:HB2	1:D:223:TYR:CD1	2.55	0.41
2:E:323:VAL:HG23	2:E:324:TYR:HD2	1.85	0.41
1:A:13:LEU:HD12	1:A:82:VAL:O	2.21	0.41
1:A:37:ASN:O	1:A:81:ASN:HB2	2.20	0.41
1:A:127:CYS:HA	1:A:129:GLN:NE2	2.35	0.41
1:A:146:LEU:O	1:A:150:LYS:HB2	2.21	0.41
2:B:343:GLY:HA2	2:B:346:ARG:HB3	2.03	0.41
3:C:133:PHE:HB2	3:C:144:ILE:HG12	2.03	0.41
1:D:59:PHE:HE1	1:D:63:ARG:CZ	2.33	0.41
2:B:131:LEU:HD12	2:B:131:LEU:HA	1.89	0.41
2:B:150:LEU:HA	2:B:150:LEU:HD23	1.81	0.41
2:E:25:THR:C	2:E:26:ILE:HD13	2.46	0.41
3:F:63:ASN:O	3:F:64:GLN:C	2.64	0.41
3:F:181:TYR:HB2	3:F:185:THR:HG21	2.03	0.41
2:B:81:VAL:HG12	2:B:87:LYS:HA	2.03	0.40
2:B:191:ILE:HA	2:B:191:ILE:HD13	1.74	0.40
3:C:19:ASN:OD1	3:C:19:ASN:C	2.65	0.40
3:C:205:VAL:HA	3:C:206:PRO:HD2	1.92	0.40
3:C:228:LYS:HE3	3:C:232:GLU:OE2	2.21	0.40
1:D:265:ASN:HD21	1:D:291:GLN:HB3	1.86	0.40
2:E:72:HIS:ND1	2:E:77:ASP:HB3	2.36	0.40
3:F:261:LEU:HA	3:F:261:LEU:HD23	1.80	0.40
1:A:10:PHE:O	3:C:311:ARG:NH2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:MET:HE3	1:D:71:SER:HB3	2.02	0.40
2:B:75:LEU:HD12	2:B:104:HIS:CD2	2.56	0.40
2:E:278:TYR:HB3	2:E:279:PRO:HD3	2.03	0.40
2:E:310:PRO:HB3	2:E:352:TRP:CE2	2.57	0.40
3:F:58:LEU:HD13	3:F:68:GLN:HG3	2.03	0.40
1:A:30:TYR:CE1	2:B:374:LYS:HB3	2.56	0.40
2:B:24:PRO:HA	2:B:380:ARG:HH21	1.85	0.40
3:C:129:SER:HB2	3:C:130:LYS:HD3	2.03	0.40
3:C:336:LEU:HD12	3:C:339:VAL:CG2	2.52	0.40
1:D:119:LEU:HD23	1:D:119:LEU:HA	1.93	0.40
2:E:253:LEU:HD12	2:E:301:ARG:NE	2.36	0.40
3:F:135:MET:HG2	8:F:616:HOH:O	2.20	0.40
1:A:181:ILE:HA	1:A:226:ILE:O	2.22	0.40
2:B:121:LEU:HD13	2:B:231:PHE:CE2	2.57	0.40
3:C:406:VAL:HG13	3:C:409:THR:OG1	2.21	0.40
1:D:263:LYS:O	1:D:266:ILE:HG22	2.22	0.40
3:F:48:VAL:HG11	3:F:79:ILE:HG12	2.02	0.40
3:F:308:LEU:C	3:F:310:GLU:H	2.29	0.40
3:C:263:MET:HE3	3:C:288:TYR:HD1	1.87	0.40
3:C:402:ILE:HG13	3:C:431:VAL:HG21	2.04	0.40
3:F:228:LYS:HE3	3:F:232:GLU:OE2	2.22	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	309/312 (99%)	267 (86%)	35 (11%)	7 (2%)	5	25
1	D	309/312 (99%)	266 (86%)	38 (12%)	5 (2%)	7	31
2	B	392/394 (100%)	359 (92%)	31 (8%)	2 (0%)	24	55
2	E	391/394 (99%)	359 (92%)	31 (8%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	420/436 (96%)	384 (91%)	32 (8%)	4 (1%)	12	40
3	F	418/436 (96%)	386 (92%)	28 (7%)	4 (1%)	12	40
All	All	2239/2284 (98%)	2021 (90%)	195 (9%)	23 (1%)	12	40

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	127	CYS
1	A	132	LYS
3	C	185	THR
3	C	188	ASP
1	D	90	SER
2	E	90	HIS
3	C	103	GLU
1	D	55	LEU
3	F	185	THR
3	F	313	GLU
1	A	125	LYS
2	B	90	HIS
1	D	163	LYS
1	A	126	ARG
1	A	153	PHE
1	A	91	LEU
3	C	186	TYR
1	D	125	LYS
2	B	180	ALA
3	F	188	ASP
3	F	315	ASP
1	D	237	GLU

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	282/283 (100%)	267 (95%)	15 (5%)	20	49
1	D	282/283 (100%)	264 (94%)	18 (6%)	16	44
2	B	358/358 (100%)	342 (96%)	16 (4%)	24	53
2	E	357/358 (100%)	341 (96%)	16 (4%)	24	53
3	C	387/399 (97%)	370 (96%)	17 (4%)	25	54
3	F	385/399 (96%)	369 (96%)	16 (4%)	26	55
All	All	2051/2080 (99%)	1953 (95%)	98 (5%)	23	52

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	54	SER
1	A	87	THR
1	A	103	GLU
1	A	129	GLN
1	A	158	ILE
1	A	162	LEU
1	A	163	LYS
1	A	164	GLU
1	A	217	MET
1	A	220	GLN
1	A	239	THR
1	A	267	ILE
1	A	269	LYS
1	A	293	VAL
2	B	25	THR
2	B	76	GLU
2	B	83	ARG
2	B	84	ASN
2	B	114	LEU
2	B	137	SER
2	B	154	SER
2	B	177	VAL
2	B	189	MET
2	B	210	GLN
2	B	225	LYS
2	B	226	GLU
2	B	243	ASP
2	B	262	ASP
2	B	354	ILE

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Mol	Chain	Res	Type
2	B	364	SER
3	C	22	THR
3	C	31	LEU
3	C	65	ILE
3	C	81	ASN
3	C	86	GLU
3	C	109	VAL
3	C	126	THR
3	C	160	SER
3	C	161	VAL
3	C	187	ILE
3	C	201	ASN
3	C	212	LEU
3	C	247	THR
3	C	283	ARG
3	C	313	GLU
3	C	315	ASP
3	C	336	LEU
1	D	62	GLU
1	D	65	THR
1	D	69	GLU
1	D	84	ILE
1	D	103	GLU
1	D	114	LEU
1	D	132	LYS
1	D	162	LEU
1	D	164	GLU
1	D	174	THR
1	D	191	LEU
1	D	239	THR
1	D	240	GLU
1	D	267	ILE
1	D	269	LYS
1	D	279	LYS
1	D	282	VAL
1	D	295	MET
2	E	9	LYS
2	E	19	ILE
2	E	56	ILE
2	E	76	GLU
2	E	114	LEU
2	E	148	GLU

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Mol	Chain	Res	Type
2	E	154	SER
2	E	177	VAL
2	E	189	MET
2	E	217	LYS
2	E	243	ASP
2	E	249	VAL
2	E	267	GLN
2	E	290	GLN
2	E	296	VAL
2	E	354	ILE
3	F	31	LEU
3	F	75	VAL
3	F	77	LEU
3	F	81	ASN
3	F	86	GLU
3	F	109	VAL
3	F	142	ILE
3	F	160	SER
3	F	161	VAL
3	F	193	GLN
3	F	247	THR
3	F	267	ILE
3	F	283	ARG
3	F	300	SER
3	F	336	LEU
3	F	337	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	192	ASN
1	A	221	GLN
2	B	20	ASN
2	B	36	ASN
2	B	219	GLN
2	B	265	HIS
2	B	333	GLN
2	B	350	ASN
3	C	4	GLN
3	C	39	ASN
3	C	89	GLN

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Mol	Chain	Res	Type
3	C	97	GLN
3	C	390	HIS
3	C	396	GLN
1	D	5	ASN
1	D	9	HIS
1	D	42	ASN
1	D	172	GLN
1	D	192	ASN
1	D	259	ASN
1	D	291	GLN
2	E	84	ASN
2	E	93	GLN
2	E	134	ASN
2	E	146	HIS
2	E	152	GLN
2	E	196	GLN
2	E	265	HIS
3	F	11	HIS
3	F	33	ASN
3	F	68	GLN
3	F	89	GLN
3	F	193	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	F	502	-	4,4,4	0.23	0	6,6,6	0.18	0
7	GOL	C	502	-	5,5,5	0.30	0	5,5,5	0.43	0
6	SO4	E	402	-	4,4,4	0.20	0	6,6,6	0.30	0
6	SO4	B	403	-	4,4,4	0.16	0	6,6,6	0.59	0
6	SO4	A	403	-	4,4,4	0.30	0	6,6,6	0.19	0
6	SO4	A	404	-	4,4,4	0.28	0	6,6,6	0.09	0
6	SO4	F	501	-	4,4,4	0.24	0	6,6,6	0.35	0
7	GOL	C	503	-	5,5,5	0.44	0	5,5,5	0.28	0
7	GOL	C	504	-	5,5,5	0.59	0	5,5,5	0.36	0
4	PO4	D	401	-	4,4,4	1.12	0	6,6,6	0.29	0
7	GOL	F	503	-	5,5,5	0.57	0	5,5,5	0.35	0
6	SO4	E	401	-	4,4,4	0.25	0	6,6,6	0.41	0
4	PO4	A	401	-	4,4,4	0.95	0	6,6,6	0.67	0
7	GOL	B	404	-	5,5,5	0.60	0	5,5,5	1.06	0
6	SO4	C	501	-	4,4,4	0.32	0	6,6,6	0.15	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
7	GOL	C	502	-	-	2/4/4/4	-
7	GOL	C	503	-	-	4/4/4/4	-
7	GOL	C	504	-	-	2/4/4/4	-
7	GOL	F	503	-	-	2/4/4/4	-
7	GOL	B	404	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	502	GOL	O1-C1-C2-C3
7	C	504	GOL	C1-C2-C3-O3
7	F	503	GOL	O1-C1-C2-C3
7	B	404	GOL	C1-C2-C3-O3
7	C	503	GOL	O1-C1-C2-C3
7	C	503	GOL	C1-C2-C3-O3
7	B	404	GOL	O2-C2-C3-O3
7	C	502	GOL	O1-C1-C2-O2
7	C	503	GOL	O2-C2-C3-O3
7	F	503	GOL	O1-C1-C2-O2
7	C	504	GOL	O2-C2-C3-O3
7	C	503	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	502	GOL	1	0
6	B	403	SO4	1	0
7	C	503	GOL	1	0
7	F	503	GOL	2	0
4	A	401	PO4	2	0
7	B	404	GOL	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	311/312 (99%)	-0.31	0 100 100	38, 77, 131, 191	0
1	D	311/312 (99%)	-0.26	3 (0%) 79 63	46, 75, 126, 167	0
2	B	394/394 (100%)	-0.59	0 100 100	35, 53, 91, 126	0
2	E	393/394 (99%)	-0.27	1 (0%) 90 82	44, 77, 118, 137	0
3	C	424/436 (97%)	-0.52	5 (1%) 76 58	35, 60, 103, 148	0
3	F	422/436 (96%)	-0.50	3 (0%) 84 70	40, 60, 98, 158	0
All	All	2255/2284 (98%)	-0.42	12 (0%) 87 76	35, 66, 115, 191	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	313	GLU	2.8
3	C	377	PHE	2.6
3	F	185	THR	2.5
1	D	263	LYS	2.4
1	D	89	SER	2.4
3	C	91	LYS	2.2
2	E	131	LEU	2.2
3	F	390	HIS	2.2
3	C	185	THR	2.1
3	C	186	TYR	2.1
3	C	101	TRP	2.1
1	D	265	ASN	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](#)

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
7	GOL	C	503	6/6	0.51	0.16	83,87,95,96	0
6	SO4	A	404	5/5	0.74	0.10	168,169,171,171	0
5	MG	B	401	1/1	0.76	0.12	42,42,42,42	0
6	SO4	F	501	5/5	0.80	0.15	135,139,140,141	0
6	SO4	A	403	5/5	0.81	0.24	143,148,149,150	0
6	SO4	C	501	5/5	0.87	0.22	125,126,127,129	0
7	GOL	C	504	6/6	0.87	0.17	53,67,72,75	0
6	SO4	E	401	5/5	0.88	0.27	123,124,126,127	0
6	SO4	F	502	5/5	0.88	0.28	135,137,143,144	0
6	SO4	B	403	5/5	0.90	0.09	70,70,73,74	0
7	GOL	B	404	6/6	0.90	0.18	55,68,75,81	0
4	PO4	D	401	5/5	0.93	0.07	56,60,68,71	0
6	SO4	E	402	5/5	0.94	0.06	90,93,95,97	0
7	GOL	C	502	6/6	0.95	0.11	73,78,80,83	0
7	GOL	F	503	6/6	0.95	0.09	56,67,74,77	0
4	PO4	A	401	5/5	0.96	0.06	51,58,62,71	0
5	MG	B	402	1/1	0.97	0.25	41,41,41,41	0
5	MG	A	402	1/1	0.97	0.13	58,58,58,58	0
5	MG	D	402	1/1	0.98	0.10	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.