



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:57 AM UTC

PDB ID : 4OL8 / pdb_00004ol8
Title : Ty3 reverse transcriptase bound to DNA/RNA
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Deposited on : 2014-01-23
Resolution : 3.10 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

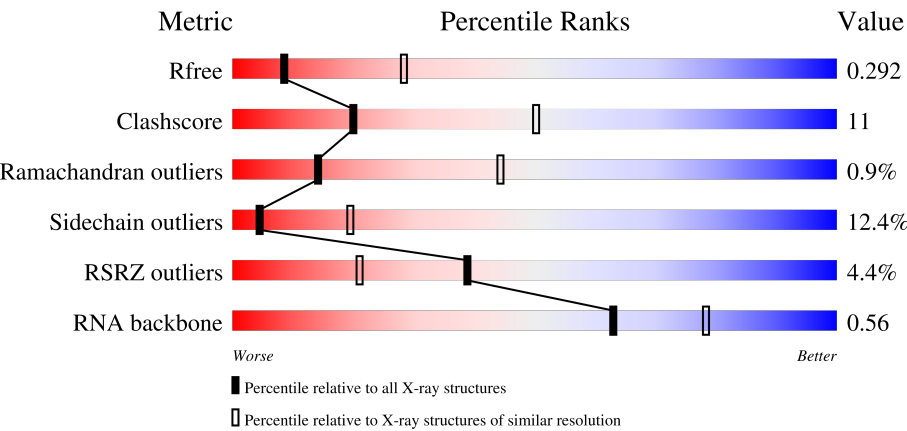
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	478	3% 53% 24% • 18%
1	B	478	• 62% 26% 6% 5%
1	E	478	9% 49% 27% • 20%
1	F	478	3% 68% 19% • 11%

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Mol	Chain	Length	Quality of chain
2	C	18	72%22%6%
2	G	18	61%28%6%6%
3	D	16	56%38%6%
3	H	16	56%44%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14105 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	Se	0	0	0
			3004	1938	504	552	5	5			
1	B	452	Total	C	N	O	S	Se	0	0	0
			3547	2291	604	639	8	5			
1	F	427	Total	C	N	O	S	Se	0	0	0
			3310	2129	561	608	7	5			
1	E	381	Total	C	N	O	S	Se	0	0	0
			2873	1839	484	540	5	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q99315
A	0	PRO	-	expression tag	UNP Q99315
A	426	ASN	ASP	engineered mutation	UNP Q99315
B	-1	GLY	-	expression tag	UNP Q99315
B	0	PRO	-	expression tag	UNP Q99315
B	426	ASN	ASP	engineered mutation	UNP Q99315
F	-1	GLY	-	expression tag	UNP Q99315
F	0	PRO	-	expression tag	UNP Q99315
F	426	ASN	ASP	engineered mutation	UNP Q99315
E	-1	GLY	-	expression tag	UNP Q99315
E	0	PRO	-	expression tag	UNP Q99315
E	426	ASN	ASP	engineered mutation	UNP Q99315

- Molecule 2 is a RNA chain called 5'-R(*CP*UP*GP*AP*GP*AP*GP*AP*GP*AP*GP*GP*AP*AP*GP*AP*UP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	P	0	0	0
			378	168	79	114	17			

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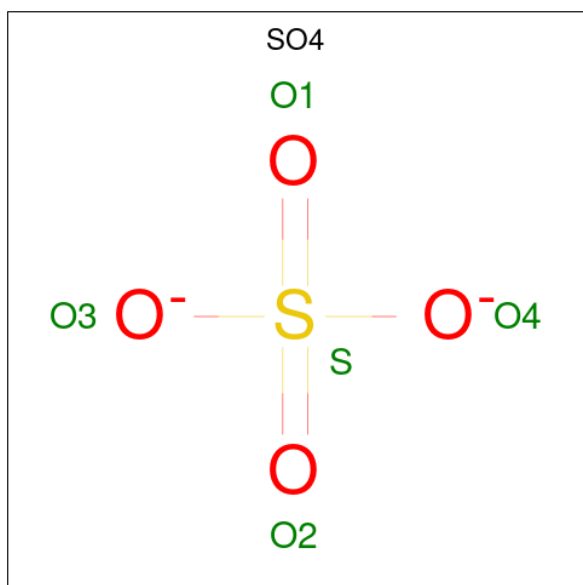
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	17	Total	C	N	O	P	0	0	0
			378	168	79	114	17			

- Molecule 3 is a DNA chain called 5'-D(*CP*AP*TP*CP*TP*TP*CP*CP*TP*CP*TP*CP*TP*CP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	15	Total	C	N	O	P	0	0	0
			294	143	40	96	15			
3	H	16	Total	C	N	O	P	0	0	0
			310	152	43	100	15			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

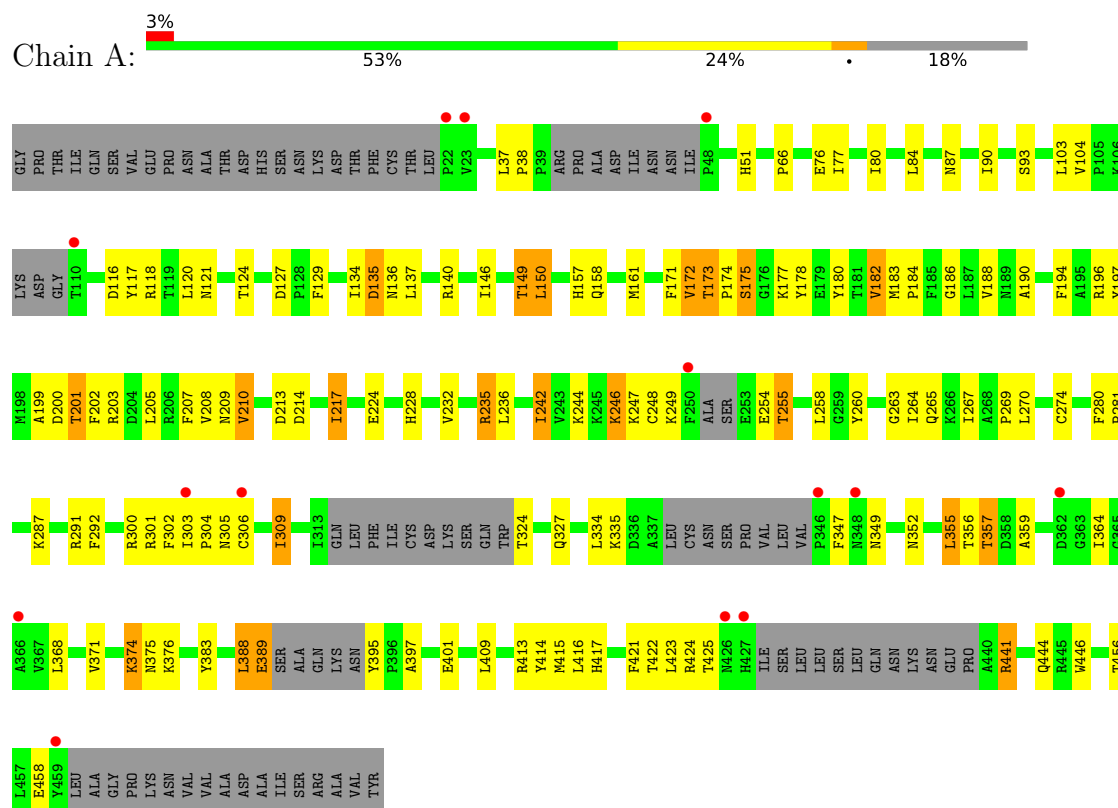
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			1	1		

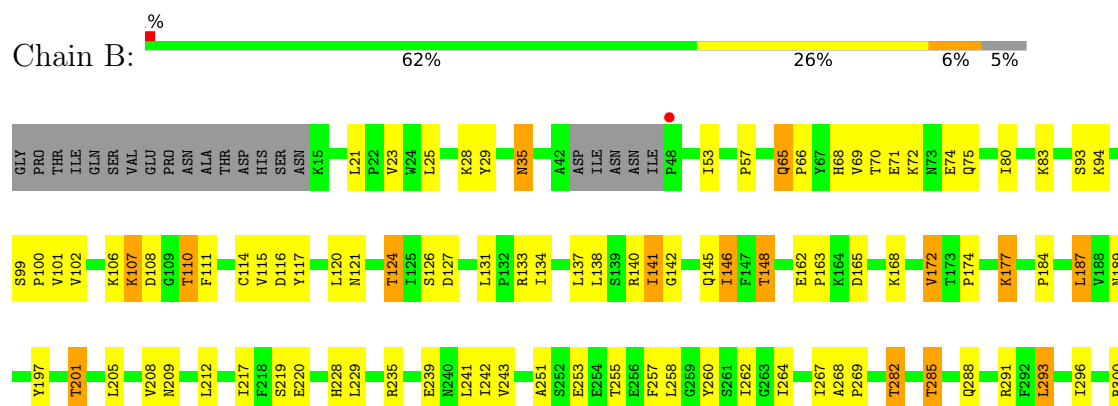
3 Residue-property plots

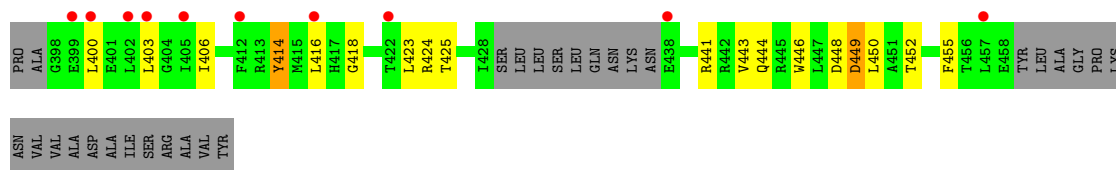
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Reverse transcriptase/ribonuclease H



• Molecule 1: Reverse transcriptase/ribonuclease H





- Molecule 2: 5'-R(*CP*UP*GP*AP*GP*AP*GP*AP*GP*AP*GP*GP*AP*AP*GP*AP*UP*G)-3'

Chain C: 72% 22% 6%



- Molecule 2: 5'-R(*CP*UP*GP*AP*GP*AP*GP*AP*GP*AP*GP*GP*AP*AP*GP*AP*UP*G)-3'

Chain G: 61% 28% 6% 6%



- Molecule 3: 5'-D(*CP*AP*TP*CP*TP*TP*CP*CP*TP*CP*TP*CP*TP*CP*TP*C)-3'

Chain D: 56% 38% 6%



- Molecule 3: 5'-D(*CP*AP*TP*CP*TP*TP*CP*CP*TP*CP*TP*CP*TP*CP*TP*C)-3'

Chain H: 56% 44%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	320.70Å 75.06Å 108.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 3.10 48.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.90-3.10) 99.7 (48.90-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.227 , 0.296 0.228 , 0.292	Depositor DCC
R_{free} test set	2665 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 105.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14105	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/3069	0.89	10/4169 (0.2%)
1	B	0.54	0/3629	0.97	13/4928 (0.3%)
1	E	0.40	0/2933	0.87	2/3990 (0.1%)
1	F	0.38	0/3382	0.84	4/4597 (0.1%)
2	C	0.20	0/426	0.34	0/665
2	G	0.19	0/426	0.33	0/665
3	D	0.24	0/324	0.78	0/495
3	H	0.23	0/342	0.72	0/523
All	All	0.43	0/14531	0.86	29/20032 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	VAL	N-CA-C	-6.98	106.69	113.53
1	B	268	ALA	CA-C-N	6.92	126.95	119.89
1	B	268	ALA	C-N-CA	6.92	126.95	119.89
1	B	21	LEU	CA-C-N	6.23	127.62	119.84
1	B	21	LEU	C-N-CA	6.23	127.62	119.84
1	B	363	GLY	N-CA-C	6.22	122.92	110.97
1	F	77	ILE	N-CA-C	-6.15	105.83	111.67
1	A	395	TYR	CA-C-N	6.05	126.07	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	TYR	C-N-CA	6.05	126.07	119.89
1	A	104	VAL	N-CA-C	5.92	115.03	108.05
1	A	173	THR	N-CA-C	-5.81	103.34	110.31
1	B	282	THR	CA-C-N	5.78	125.74	119.78
1	B	282	THR	C-N-CA	5.78	125.74	119.78
1	F	20	THR	N-CA-C	-5.77	107.23	114.56
1	E	139	SER	N-CA-C	-5.63	104.65	112.30
1	B	94	LYS	N-CA-C	-5.56	104.03	111.87
1	A	104	VAL	CA-C-N	5.42	125.62	120.31
1	A	104	VAL	C-N-CA	5.42	125.62	120.31
1	A	375	ASN	N-CA-C	5.42	115.70	108.23
1	F	162	GLU	CA-C-N	5.22	125.27	119.32
1	F	162	GLU	C-N-CA	5.22	125.27	119.32
1	A	190	ALA	CA-C-N	-5.19	113.19	118.85
1	A	190	ALA	C-N-CA	-5.19	113.19	118.85
1	B	303	ILE	CA-C-N	5.17	126.30	119.84
1	B	303	ILE	C-N-CA	5.17	126.30	119.84
1	B	93	SER	N-CA-C	5.10	117.61	109.81
1	B	464	LYS	N-CA-C	-5.03	107.82	114.31
1	E	158	GLN	N-CA-C	-5.02	107.29	113.41
1	A	441	ARG	N-CA-C	5.00	116.42	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	475	VAL	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	3004	0	2838	85	0
1	B	3547	0	3500	85	0
1	E	2873	0	2637	88	0
1	F	3310	0	3193	50	0
2	C	378	0	186	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	378	0	186	6	0
3	D	294	0	173	6	0
3	H	310	0	185	8	0
4	B	10	0	0	1	0
5	B	1	0	0	0	0
All	All	14105	0	12898	308	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 11.

All (308) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:SER:HB3	1:E:157:HIS:HB2	1.57	0.86
1:B:148:THR:HG1	1:B:251:ALA:H	1.29	0.80
1:F:50:LYS:HG2	1:F:160:PRO:HG2	1.67	0.76
1:B:205:LEU:HD21	1:B:235:ARG:HH12	1.51	0.75
1:A:349:ASN:HD21	1:B:72:LYS:HE3	1.50	0.75
1:E:153:HIS:HB3	1:E:244:LYS:HB2	1.68	0.73
1:F:364:ILE:HG12	1:F:404:GLY:HA3	1.69	0.73
1:E:141:ILE:HB	1:E:346:PRO:HB3	1.69	0.73
1:E:285:THR:H	1:E:288:GLN:HE22	1.35	0.72
1:A:199:ALA:O	1:A:203:ARG:HB2	1.92	0.69
1:B:376:LYS:HD2	1:B:377:LEU:H	1.58	0.68
2:G:16:A:H2	3:H:34:DT:H3	1.40	0.67
1:F:80:ILE:HD11	1:F:111:PHE:HB2	1.76	0.67
1:E:137:LEU:O	1:E:209:ASN:ND2	2.28	0.67
1:F:108:ASP:OD1	1:F:108:ASP:N	2.27	0.67
1:E:138:LEU:HD12	1:E:301:ARG:HH22	1.59	0.66
1:B:291:ARG:NH2	4:B:501:SO4:O2	2.29	0.66
1:F:348:ASN:HB3	1:F:351:ALA:HB2	1.76	0.66
1:A:161:MSE:HE3	1:A:184:PRO:HD2	1.76	0.66
1:E:357:THR:O	1:E:357:THR:OG1	2.13	0.65
1:A:388:LEU:HB2	1:A:389:GLU:HB2	1.78	0.64
1:B:219:SER:OG	1:B:228:HIS:ND1	2.29	0.64
3:H:45:DC:H4'	1:E:298:TYR:CD2	2.32	0.64
1:E:262:ILE:HG23	1:E:267:ILE:HG12	1.80	0.64
1:E:204:ASP:OD1	1:E:204:ASP:N	2.30	0.64
2:G:2:U:H1'	1:E:114:CYS:SG	2.38	0.63
1:B:370:GLU:HB3	1:B:378:VAL:HG22	1.81	0.63
1:A:77:ILE:HG13	1:A:103:LEU:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:449:ASP:N	1:E:449:ASP:OD1	2.28	0.62
1:A:140:ARG:NH1	1:B:71:GLU:OE1	2.32	0.62
1:A:359:ALA:N	1:A:401:GLU:OE2	2.32	0.62
1:A:200:ASP:OD1	1:A:203:ARG:NH2	2.26	0.62
1:B:107:LYS:HE3	1:B:107:LYS:H	1.63	0.62
1:B:436:LYS:NZ	3:D:38:DC:OP2	2.31	0.62
1:E:285:THR:N	1:E:288:GLN:HE22	1.97	0.62
1:E:144:ALA:HA	1:E:220:GLU:HA	1.80	0.62
1:B:300:ARG:HH22	1:B:307:SER:HB3	1.65	0.61
1:A:356:THR:HG22	1:A:424:ARG:HB2	1.81	0.61
1:B:148:THR:HG1	1:B:251:ALA:N	1.97	0.61
1:A:129:PHE:CE2	1:A:196:ARG:HG3	2.36	0.60
1:B:425:THR:HG21	1:B:430:LEU:HD13	1.82	0.60
3:H:37:DT:H2'	3:H:38:DC:H6	1.66	0.60
1:E:145:GLN:HG3	1:E:264:ILE:HD11	1.83	0.60
1:B:462:GLY:HA2	1:B:464:LYS:H	1.67	0.60
1:B:102:VAL:HG23	1:B:114:CYS:HB3	1.84	0.60
1:A:134:ILE:HG23	1:A:258:LEU:HD13	1.83	0.60
1:B:126:SER:HA	1:B:189:ASN:OD1	2.03	0.59
1:A:444:GLN:HB3	1:B:428:ILE:HD12	1.84	0.59
1:E:264:ILE:HG23	1:E:265:GLN:H	1.66	0.59
1:A:397:ALA:O	1:A:401:GLU:N	2.35	0.59
1:E:297:ASN:O	1:E:300:ARG:HG2	2.03	0.59
1:B:312:PRO:O	1:B:327:GLN:NE2	2.36	0.59
1:F:75:GLN:OE1	1:E:206:ARG:NE	2.35	0.59
1:A:287:LYS:O	1:A:291:ARG:N	2.28	0.58
1:B:293:LEU:HD21	1:B:310:ALA:HB1	1.83	0.58
1:B:449:ASP:N	1:B:449:ASP:OD1	2.35	0.58
1:E:254:GLU:HA	1:E:263:GLY:HA2	1.85	0.58
1:E:256:GLU:HA	1:E:261:SER:HA	1.83	0.58
1:B:165:ASP:OD1	1:B:168:LYS:NZ	2.25	0.58
1:E:143:ASN:N	1:E:143:ASN:OD1	2.36	0.58
1:A:260:TYR:OH	1:A:301:ARG:NH2	2.37	0.58
1:F:133:ARG:HD3	1:F:136:ASN:HB3	1.86	0.57
1:F:353:TYR:HE1	1:F:381:VAL:HG21	1.68	0.57
1:A:300:ARG:NH1	1:A:306:CYS:SG	2.78	0.57
3:H:37:DT:H2'	3:H:38:DC:C6	2.39	0.57
1:E:219:SER:HB3	1:E:228:HIS:ND1	2.19	0.57
1:E:262:ILE:HG12	1:E:267:ILE:HG23	1.86	0.57
1:A:249:LYS:HD2	1:A:255:THR:HG23	1.86	0.56
1:F:146:ILE:HG21	1:F:225:HIS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:TYR:CE1	1:F:269:PRO:HB3	2.40	0.56
3:D:45:DC:H2'	3:D:46:DT:C6	2.40	0.56
1:B:134:ILE:HG12	1:B:258:LEU:HD23	1.86	0.56
1:A:292:PHE:CE1	1:A:334:LEU:HD11	2.41	0.56
1:F:427:HIS:CE1	1:F:429:SER:HB3	2.41	0.56
1:B:74:GLU:HG3	1:B:174:PRO:HG2	1.88	0.56
1:E:150:LEU:HD12	1:E:243:VAL:HG11	1.87	0.55
1:E:156:TYR:CD2	1:E:183:MSE:HE3	2.41	0.55
1:B:362:ASP:O	1:B:388:LEU:N	2.39	0.55
1:F:146:ILE:HD11	1:F:251:ALA:HB1	1.87	0.55
1:F:200:ASP:OD1	1:F:203:ARG:NH2	2.40	0.55
1:A:309:ILE:HD11	1:A:334:LEU:HD23	1.88	0.55
1:A:173:THR:HG23	1:A:175:SER:H	1.72	0.54
1:A:347:PHE:CD1	1:A:415:MSE:HE3	2.43	0.54
1:E:355:LEU:HD13	1:E:416:LEU:HD21	1.89	0.54
1:B:296:ILE:HG21	1:B:334:LEU:HD22	1.89	0.54
1:B:106:LYS:HD3	1:B:110:THR:HB	1.90	0.54
1:B:100:PRO:HG2	1:B:116:ASP:HB3	1.91	0.54
1:A:116:ASP:OD2	1:A:118:ARG:NH1	2.41	0.53
1:A:186:GLY:HA2	2:C:3:G:O4'	2.08	0.53
1:B:416:LEU:HD22	1:B:421:PHE:CD1	2.43	0.53
1:A:157:HIS:HA	1:A:182:VAL:HG13	1.90	0.53
1:F:31:GLU:HG3	1:F:32:ILE:HG23	1.89	0.53
1:F:148:THR:OG1	1:F:225:HIS:NE2	2.37	0.53
1:E:66:PRO:HG3	1:E:172:VAL:HB	1.90	0.53
1:A:136:ASN:O	1:A:140:ARG:HG3	2.09	0.53
1:B:148:THR:OG1	1:B:251:ALA:N	2.25	0.53
1:F:77:ILE:HG23	1:F:113:LEU:HD21	1.90	0.53
1:F:260:TYR:HA	1:F:269:PRO:HA	1.90	0.53
1:A:196:ARG:O	1:A:199:ALA:N	2.42	0.53
1:B:314:GLN:O	1:B:318:CYS:HB2	2.08	0.53
1:E:297:ASN:HA	1:E:300:ARG:HD3	1.91	0.52
1:A:202:PHE:HB2	1:A:210:VAL:HG11	1.91	0.52
1:A:84:LEU:HB3	1:A:90:ILE:HG12	1.90	0.52
1:E:89:PHE:O	1:E:181:THR:OG1	2.27	0.52
1:B:131:LEU:HD21	1:B:212:LEU:HG	1.92	0.52
1:A:134:ILE:HD12	1:A:134:ILE:H	1.75	0.52
1:A:172:VAL:HG13	1:A:177:LYS:HG3	1.92	0.52
1:A:161:MSE:HE3	1:A:183:MSE:HA	1.91	0.52
1:B:262:ILE:HD13	1:B:267:ILE:HG13	1.91	0.52
1:A:127:ASP:OD2	1:A:196:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HG22	1:A:180:TYR:HA	1.91	0.51
1:E:152:LEU:HD21	1:E:158:GLN:HB2	1.93	0.51
1:A:207:PHE:CD1	1:A:208:VAL:HG23	2.45	0.51
1:E:199:ALA:O	1:E:203:ARG:HB2	2.11	0.51
1:A:359:ALA:HB1	1:A:364:ILE:HA	1.93	0.51
1:F:163:PRO:HA	1:F:166:ARG:HD3	1.91	0.51
1:A:413:ARG:NH1	1:B:68:HIS:HB2	2.26	0.51
1:E:285:THR:H	1:E:288:GLN:NE2	2.07	0.51
1:F:106:LYS:HE3	1:F:112:ARG:HD3	1.93	0.50
1:E:82:GLN:HG3	1:E:85:LEU:HD12	1.91	0.50
1:A:303:ILE:HB	1:A:306:CYS:HB2	1.93	0.50
1:B:208:VAL:HG22	1:B:217:ILE:HG12	1.93	0.50
1:B:106:LYS:C	1:B:108:ASP:H	2.19	0.50
2:G:16:A:N1	3:H:34:DT:O4	2.45	0.50
1:A:356:THR:HG22	1:A:424:ARG:HD3	1.94	0.50
1:A:158:GLN:OE1	1:A:242:ILE:N	2.45	0.49
1:F:50:LYS:HD3	1:F:163:PRO:HD3	1.94	0.49
1:E:414:TYR:H	1:E:414:TYR:HD1	1.60	0.49
1:A:246:LYS:HZ3	1:A:246:LYS:HB3	1.77	0.49
1:B:65:GLN:HG3	1:B:66:PRO:HD2	1.93	0.49
1:F:429:SER:HB2	1:E:448:ASP:OD2	2.12	0.49
1:A:254:GLU:HG3	1:A:263:GLY:HA2	1.92	0.49
1:B:110:THR:HG22	1:B:111:PHE:H	1.78	0.49
1:E:216:LEU:HG	1:E:217:ILE:N	2.27	0.49
1:E:423:LEU:HD13	1:E:424:ARG:N	2.28	0.48
1:A:149:THR:HG22	1:A:248:CYS:HB2	1.94	0.48
2:G:2:U:H5'	1:E:118:ARG:HH21	1.79	0.48
1:F:145:GLN:HA	1:F:264:ILE:HB	1.94	0.48
1:E:100:PRO:HG2	1:E:116:ASP:HB3	1.96	0.48
1:F:277:ILE:HD13	1:F:295:MSE:HE1	1.95	0.48
1:E:110:THR:OG1	1:E:111:PHE:N	2.45	0.48
1:B:53:ILE:HB	1:B:168:LYS:HD3	1.96	0.48
1:B:184:PRO:HG2	1:B:187:LEU:HD22	1.94	0.48
3:H:32:DC:H2'	3:H:33:DA:C8	2.48	0.48
1:E:141:ILE:HA	1:E:218:PHE:CZ	2.49	0.48
1:A:118:ARG:NH2	2:C:2:U:H5''	2.29	0.47
1:A:368:LEU:HD21	1:A:416:LEU:HD21	1.96	0.47
1:F:102:VAL:HG11	1:F:444:GLN:HB3	1.96	0.47
1:B:338:LEU:HA	1:B:343:VAL:HG11	1.96	0.47
1:E:95:SER:HB2	1:E:167:TYR:HB2	1.96	0.47
1:F:352:ASN:HB2	1:F:371:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TYR:O	1:A:121:ASN:ND2	2.47	0.47
1:A:292:PHE:HE1	1:A:334:LEU:HD11	1.78	0.47
1:B:28:LYS:HD3	1:B:29:TYR:CZ	2.50	0.47
1:E:309:ILE:HD11	1:E:333:LYS:HB2	1.97	0.47
1:A:304:PRO:HB3	1:A:383:TYR:CD2	2.49	0.47
1:B:235:ARG:O	1:B:239:GLU:HG2	2.14	0.47
1:F:372:ASP:OD1	1:F:372:ASP:N	2.45	0.47
1:E:121:ASN:C	1:E:123:ALA:H	2.22	0.47
1:A:357:THR:O	1:A:357:THR:OG1	2.31	0.47
1:B:306:CYS:HA	1:B:309:ILE:HG22	1.97	0.47
1:F:428:ILE:HG12	1:E:444:GLN:HB3	1.97	0.47
1:A:135:ASP:OD1	1:A:414:TYR:OH	2.30	0.47
1:A:183:MSE:HE1	1:A:194:PHE:HB2	1.95	0.47
1:B:205:LEU:HD21	1:B:235:ARG:NH1	2.26	0.47
1:B:344:LEU:HD23	1:B:380:VAL:O	2.15	0.47
1:E:306:CYS:O	1:E:309:ILE:HG22	2.15	0.47
1:A:304:PRO:HB3	1:A:383:TYR:CE2	2.50	0.46
1:F:311:GLN:H	1:F:312:PRO:HD2	1.80	0.46
1:A:352:ASN:OD1	1:A:352:ASN:N	2.47	0.46
1:B:131:LEU:CD2	1:B:212:LEU:HG	2.46	0.46
1:E:146:ILE:HD11	1:E:229:LEU:HD21	1.96	0.46
1:F:428:ILE:HA	1:F:431:LEU:HB2	1.96	0.46
1:B:260:TYR:HA	1:B:269:PRO:HA	1.98	0.46
3:H:44:DT:H4'	1:E:294:GLY:C	2.41	0.46
1:B:138:LEU:HD22	1:B:262:ILE:HD11	1.97	0.46
1:E:35:ASN:OD1	1:E:245:LYS:N	2.48	0.46
3:D:44:DT:H2'	3:D:45:DC:C6	2.51	0.46
1:A:355:LEU:HB3	1:A:423:LEU:HD23	1.98	0.46
1:A:417:HIS:O	1:B:70:THR:HG21	2.16	0.46
1:F:336:ASP:OD1	1:F:336:ASP:N	2.50	0.46
1:A:305:ASN:O	1:A:309:ILE:HG23	2.16	0.45
2:G:4:A:H2'	2:G:5:G:O4'	2.16	0.45
1:B:172:VAL:HG23	1:B:177:LYS:HG2	1.97	0.45
3:D:38:DC:H2'	3:D:39:DC:H6	1.81	0.45
1:E:55:ILE:HG12	1:E:124:THR:HG22	1.98	0.45
1:E:64:LEU:HD12	1:E:100:PRO:HD3	1.97	0.45
1:B:402:LEU:HD13	1:B:446:TRP:CD1	2.51	0.45
1:A:423:LEU:O	1:A:458:GLU:N	2.50	0.45
1:B:141:ILE:HG13	1:B:142:GLY:N	2.31	0.45
1:B:172:VAL:HG23	1:B:177:LYS:CG	2.47	0.45
1:F:280:PHE:HA	1:F:281:PRO:HD3	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:GLU:HG2	1:B:371:VAL:H	1.81	0.45
1:B:285:THR:HB	1:B:288:GLN:HG3	1.97	0.45
1:F:338:LEU:HD23	1:F:343:VAL:HG11	1.97	0.45
1:E:141:ILE:HA	1:E:218:PHE:CE1	2.52	0.45
1:A:197:TYR:O	1:A:201:THR:OG1	2.32	0.45
1:A:120:LEU:O	1:A:124:THR:HG23	2.16	0.45
1:F:78:ASN:ND2	1:E:203:ARG:HD3	2.31	0.44
1:A:173:THR:OG1	1:A:174:PRO:HD2	2.15	0.44
1:E:416:LEU:O	1:E:418:GLY:HA2	2.17	0.44
1:A:374:LYS:HE3	1:A:374:LYS:HB2	1.74	0.44
1:E:291:ARG:O	1:E:295:MSE:HG3	2.17	0.44
1:A:51:HIS:HB3	1:A:161:MSE:HE2	2.00	0.44
1:A:80:ILE:HG22	1:A:84:LEU:HD23	1.99	0.44
1:B:368:LEU:O	1:B:381:VAL:HG23	2.18	0.44
1:B:476:TYR:N	1:B:476:TYR:CD1	2.85	0.44
1:E:80:ILE:HD12	1:E:80:ILE:HA	1.86	0.44
1:F:22:PRO:HB2	1:F:24:TRP:CD1	2.53	0.44
1:F:270:LEU:HD12	1:F:270:LEU:H	1.83	0.44
1:E:141:ILE:HD13	1:E:218:PHE:CD2	2.52	0.44
1:E:313:ILE:HD13	1:E:327:GLN:HB2	1.99	0.44
1:B:197:TYR:CE2	1:B:241:LEU:HD11	2.53	0.44
1:E:187:LEU:HB2	1:E:190:ALA:HB2	2.00	0.44
1:E:132:PRO:HG2	1:E:210:VAL:O	2.18	0.44
1:E:166:ARG:O	1:E:169:THR:OG1	2.35	0.44
1:E:205:LEU:HD12	1:E:207:PHE:CZ	2.52	0.44
1:B:121:ASN:HA	1:B:124:THR:HG23	1.98	0.43
1:F:244:LYS:HE2	1:F:244:LYS:HB3	1.76	0.43
1:A:173:THR:HG23	1:A:175:SER:N	2.33	0.43
1:A:376:LYS:HD3	1:A:376:LYS:HA	1.65	0.43
1:B:107:LYS:HE2	1:B:445:ARG:NH2	2.33	0.43
1:F:253:GLU:HG3	1:F:254:GLU:HG2	2.01	0.43
1:E:207:PHE:CD1	1:E:208:VAL:HG23	2.53	0.43
1:A:66:PRO:HG3	1:A:172:VAL:HB	2.00	0.43
1:B:35:ASN:OD1	1:B:35:ASN:N	2.49	0.43
1:B:257:PHE:CE2	1:B:258:LEU:HD22	2.53	0.43
1:E:55:ILE:HG23	1:E:123:ALA:O	2.18	0.43
1:A:171:PHE:CE1	1:A:178:TYR:HB2	2.54	0.43
1:B:162:GLU:HA	1:B:163:PRO:HD2	1.80	0.43
1:B:197:TYR:O	1:B:201:THR:HG23	2.19	0.43
1:A:334:LEU:HD12	1:A:335:LYS:N	2.33	0.43
1:B:115:VAL:HG11	1:B:117:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:38:DC:H2'	3:D:39:DC:C6	2.54	0.43
1:A:213:ASP:OD1	1:A:213:ASP:N	2.44	0.43
1:A:224:GLU:HG2	1:A:228:HIS:CE1	2.54	0.43
1:B:140:ARG:NH1	1:B:209:ASN:OD1	2.52	0.43
1:B:146:ILE:HD12	1:B:146:ILE:H	1.84	0.43
3:H:45:DC:H4'	1:E:298:TYR:CG	2.54	0.43
1:F:138:LEU:HD13	1:F:267:ILE:HD13	2.01	0.43
1:F:257:PHE:CE2	1:F:258:LEU:HD22	2.54	0.43
1:A:280:PHE:HA	1:A:281:PRO:HD3	1.92	0.42
1:B:293:LEU:HD23	1:B:313:ILE:HG21	2.01	0.42
1:E:81:VAL:O	1:E:85:LEU:HG	2.19	0.42
1:E:139:SER:HA	1:E:347:PHE:HB2	2.00	0.42
1:B:440:ALA:O	1:B:443:VAL:HG12	2.20	0.42
1:B:473:ARG:HB3	1:B:473:ARG:NH1	2.35	0.42
1:E:357:THR:HA	1:E:366:ALA:HA	2.01	0.42
1:F:118:ARG:NH2	1:F:439:PRO:HD3	2.34	0.42
1:F:428:ILE:CD1	1:E:448:ASP:HB2	2.50	0.42
1:E:59:ALA:HB1	1:E:123:ALA:HB1	2.01	0.42
1:E:194:PHE:O	1:E:198:MSE:HG2	2.20	0.42
1:A:37:LEU:HA	1:A:38:PRO:HD2	1.87	0.42
1:A:205:LEU:HD12	1:A:207:PHE:CZ	2.55	0.42
1:E:208:VAL:HG22	1:E:217:ILE:HB	2.02	0.42
1:E:269:PRO:HD3	1:E:302:PHE:CE2	2.55	0.42
1:B:469:ASP:OD2	1:B:473:ARG:HG3	2.19	0.42
1:E:70:THR:O	1:E:74:GLU:HB3	2.19	0.42
1:E:299:TYR:HB3	1:E:302:PHE:CD1	2.55	0.42
1:A:309:ILE:HD11	1:A:334:LEU:HB3	2.01	0.42
1:F:351:ALA:HB3	1:F:353:TYR:CE2	2.55	0.42
1:A:413:ARG:HH12	1:B:68:HIS:HB2	1.85	0.42
1:B:72:LYS:O	1:B:75:GLN:HB2	2.20	0.42
1:E:443:VAL:HA	1:E:446:TRP:CD1	2.54	0.42
1:A:409:LEU:HD21	1:A:421:PHE:HZ	1.84	0.41
1:F:441:ARG:HA	1:F:444:GLN:NE2	2.35	0.41
1:A:149:THR:O	1:A:150:LEU:HD13	2.20	0.41
1:B:138:LEU:HD13	1:B:267:ILE:HG21	2.02	0.41
1:B:313:ILE:HD11	1:B:331:ILE:HG12	2.02	0.41
1:F:170:ALA:HA	1:F:178:TYR:O	2.20	0.41
1:E:400:LEU:O	1:E:403:LEU:HB2	2.20	0.41
3:D:46:DT:H2'	3:D:47:DC:C6	2.55	0.41
1:E:146:ILE:HG12	1:E:225:HIS:CB	2.50	0.41
1:E:217:ILE:HD11	1:E:228:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:HD13	1:A:209:ASN:HB3	2.02	0.41
2:G:7:G:H2'	2:G:8:A:H8	1.86	0.41
1:B:314:GLN:HA	1:B:317:ILE:HD12	2.01	0.41
1:F:361:LYS:NZ	1:F:361:LYS:HB3	2.36	0.41
1:B:302:PHE:O	1:B:342:PRO:HD2	2.21	0.41
1:F:61:LEU:HB3	1:F:62:PRO:HD2	2.02	0.41
1:F:176:GLY:HA2	1:E:129:PHE:CZ	2.56	0.41
1:A:269:PRO:HD3	1:A:302:PHE:CZ	2.56	0.41
1:B:431:LEU:HA	1:B:457:LEU:HD13	2.02	0.41
1:F:51:HIS:HB2	1:F:193:THR:HG21	2.03	0.41
1:F:160:PRO:HA	1:F:182:VAL:HA	2.03	0.41
1:A:149:THR:OG1	1:A:255:THR:HG21	2.21	0.41
1:B:80:ILE:HA	1:B:83:LYS:HE2	2.03	0.41
1:B:107:LYS:H	1:B:107:LYS:CD	2.33	0.41
1:B:187:LEU:HD12	1:B:187:LEU:HA	1.79	0.41
1:B:374:LYS:O	1:B:376:LYS:N	2.53	0.41
1:E:307:SER:N	1:E:385:SER:OG	2.53	0.41
1:B:107:LYS:H	1:B:107:LYS:CE	2.30	0.40
1:B:427:HIS:CE1	1:B:429:SER:HB2	2.56	0.40
1:A:205:LEU:HD21	1:A:235:ARG:NH2	2.36	0.40
1:A:244:LYS:HD2	1:A:247:LYS:CG	2.52	0.40
1:E:33:ILE:HG21	1:E:250:PHE:HZ	1.87	0.40
1:E:92:PRO:HA	1:E:178:TYR:CD1	2.56	0.40
1:E:156:TYR:HD2	1:E:183:MSE:HE3	1.85	0.40
1:E:207:PHE:HB2	1:E:218:PHE:O	2.21	0.40
1:A:76:GLU:HB3	1:A:103:LEU:HD11	2.03	0.40
1:A:208:VAL:HG22	1:A:217:ILE:HB	2.02	0.40
1:A:236:LEU:HD23	1:A:236:LEU:HA	1.96	0.40
1:E:120:LEU:HD23	1:E:120:LEU:HA	1.91	0.40
1:E:230:ASP:O	1:E:234:GLU:HG3	2.21	0.40
1:B:25:LEU:HD23	1:B:25:LEU:HA	1.87	0.40
1:E:29:TYR:HB3	1:E:33:ILE:HG12	2.04	0.40
1:A:371:VAL:HG22	1:A:376:LYS:O	2.21	0.40
1:F:246:LYS:H	1:F:246:LYS:HG3	1.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	374/478 (78%)	338 (90%)	36 (10%)	0	100	100
1	B	446/478 (93%)	398 (89%)	45 (10%)	3 (1%)	18	49
1	E	361/478 (76%)	307 (85%)	45 (12%)	9 (2%)	4	21
1	F	415/478 (87%)	376 (91%)	37 (9%)	2 (0%)	24	57
All	All	1596/1912 (84%)	1419 (89%)	163 (10%)	14 (1%)	14	44

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	205	LEU
1	E	264	ILE
1	E	251	ALA
1	B	318	CYS
1	F	372	ASP
1	E	122	LYS
1	E	305	ASN
1	E	455	PHE
1	B	304	PRO
1	E	302	PHE
1	F	251	ALA
1	E	36	ASP
1	E	70	THR
1	B	57	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/426 (71%)	267 (88%)	37 (12%)	5	20
1	B	377/426 (88%)	323 (86%)	54 (14%)	3	14
1	E	286/426 (67%)	248 (87%)	38 (13%)	4	17
1	F	347/426 (82%)	313 (90%)	34 (10%)	7	29
All	All	1314/1704 (77%)	1151 (88%)	163 (12%)	4	19

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	93	SER
1	A	135	ASP
1	A	146	ILE
1	A	149	THR
1	A	150	LEU
1	A	172	VAL
1	A	175	SER
1	A	182	VAL
1	A	188	VAL
1	A	201	THR
1	A	210	VAL
1	A	214	ASP
1	A	217	ILE
1	A	232	VAL
1	A	235	ARG
1	A	242	ILE
1	A	246	LYS
1	A	255	THR
1	A	264	ILE
1	A	265	GLN
1	A	267	ILE
1	A	270	LEU
1	A	274	CYS
1	A	309	ILE
1	A	324	THR
1	A	327	GLN
1	A	355	LEU
1	A	357	THR
1	A	374	LYS
1	A	388	LEU
1	A	389	GLU
1	A	422	THR

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Mol	Chain	Res	Type
1	A	425	THR
1	A	441	ARG
1	A	446	TRP
1	A	456	THR
1	B	23	VAL
1	B	35	ASN
1	B	65	GLN
1	B	69	VAL
1	B	99	SER
1	B	101	VAL
1	B	107	LYS
1	B	110	THR
1	B	120	LEU
1	B	124	THR
1	B	127	ASP
1	B	133	ARG
1	B	137	LEU
1	B	141	ILE
1	B	145	GLN
1	B	146	ILE
1	B	148	THR
1	B	172	VAL
1	B	177	LYS
1	B	187	LEU
1	B	201	THR
1	B	220	GLU
1	B	229	LEU
1	B	242	ILE
1	B	243	VAL
1	B	253	GLU
1	B	255	THR
1	B	264	ILE
1	B	282	THR
1	B	285	THR
1	B	293	LEU
1	B	303	ILE
1	B	318	CYS
1	B	321	SER
1	B	327	GLN
1	B	331	ILE
1	B	344	LEU
1	B	356	THR

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Mol	Chain	Res	Type
1	B	364	ILE
1	B	367	VAL
1	B	371	VAL
1	B	378	VAL
1	B	380	VAL
1	B	381	VAL
1	B	400	LEU
1	B	402	LEU
1	B	403	LEU
1	B	419	LYS
1	B	428	ILE
1	B	430	LEU
1	B	442	ARG
1	B	449	ASP
1	B	466	VAL
1	B	475	VAL
1	F	21	LEU
1	F	23	VAL
1	F	60	ARG
1	F	63	ARG
1	F	69	VAL
1	F	101	VAL
1	F	108	ASP
1	F	120	LEU
1	F	136	ASN
1	F	143	ASN
1	F	152	LEU
1	F	153	HIS
1	F	154	SER
1	F	175	SER
1	F	198	MSE
1	F	212	LEU
1	F	220	GLU
1	F	231	THR
1	F	242	ILE
1	F	246	LYS
1	F	264	ILE
1	F	266	LYS
1	F	331	ILE
1	F	336	ASP
1	F	355	LEU
1	F	361	LYS

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Mol	Chain	Res	Type
1	F	375	ASN
1	F	376	LYS
1	F	386	LYS
1	F	402	LEU
1	F	419	LYS
1	F	425	THR
1	F	430	LEU
1	F	441	ARG
1	E	60	ARG
1	E	69	VAL
1	E	71	GLU
1	E	74	GLU
1	E	80	ILE
1	E	84	LEU
1	E	86	ASP
1	E	87	ASN
1	E	93	SER
1	E	104	VAL
1	E	110	THR
1	E	120	LEU
1	E	140	ARG
1	E	143	ASN
1	E	146	ILE
1	E	153	HIS
1	E	182	VAL
1	E	188	VAL
1	E	204	ASP
1	E	219	SER
1	E	248	CYS
1	E	274	CYS
1	E	288	GLN
1	E	308	LYS
1	E	309	ILE
1	E	326	LYS
1	E	327	GLN
1	E	344	LEU
1	E	356	THR
1	E	357	THR
1	E	369	GLU
1	E	406	ILE
1	E	414	TYR
1	E	425	THR

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Mol	Chain	Res	Type
1	E	441	ARG
1	E	449	ASP
1	E	450	LEU
1	E	452	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	265	GLN
1	A	349	ASN
1	B	26	GLN
1	B	327	GLN
1	B	348	ASN
1	B	411	HIS
1	B	435	ASN
1	B	437	ASN
1	F	265	GLN
1	E	87	ASN
1	E	288	GLN
1	E	311	GLN
1	E	327	GLN
1	E	411	HIS
1	E	417	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	16/18 (88%)	2 (12%)	0
2	G	16/18 (88%)	1 (6%)	0
All	All	32/36 (88%)	3 (9%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	5	G
2	C	11	G
2	G	5	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	B	502	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	B	501	-	4,4,4	0.21	0	6,6,6	0.12	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	385/478 (80%)	0.20	14 (3%) 46 26	77, 132, 173, 195	1 (0%)
1	B	447/478 (93%)	-0.16	5 (1%) 78 59	55, 87, 137, 174	2 (0%)
1	E	376/478 (78%)	0.74	42 (11%) 10 5	94, 158, 204, 236	0
1	F	422/478 (88%)	0.25	13 (3%) 51 30	75, 142, 197, 239	0
2	C	17/18 (94%)	-0.35	0 100 100	101, 147, 167, 189	0
2	G	17/18 (94%)	-0.18	0 100 100	120, 146, 202, 216	0
3	D	15/16 (93%)	0.19	0 100 100	125, 147, 196, 224	0
3	H	16/16 (100%)	0.31	0 100 100	126, 144, 216, 234	0
All	All	1695/1980 (85%)	0.23	74 (4%) 39 21	55, 132, 193, 239	3 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	ASN	4.9
1	F	158	GLN	4.4
1	F	466	VAL	4.3
1	A	23	VAL	3.8
1	E	258	LEU	3.6
1	A	48	PRO	3.3
1	A	306	CYS	3.2
1	F	460	LEU	3.2
1	E	334	LEU	3.2
1	F	312	PRO	3.2
1	E	22	PRO	3.1
1	A	366	ALA	3.1
1	E	367	VAL	3.1
1	F	356	THR	3.0
1	E	405	ILE	3.0
1	E	403	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	250	PHE	2.9
1	E	400	LEU	2.9
1	A	427	HIS	2.9
1	A	22	PRO	2.8
1	A	346	PRO	2.8
1	F	450	LEU	2.8
1	E	262	ILE	2.8
1	E	148	THR	2.7
1	E	343	VAL	2.7
1	E	385	SER	2.6
1	E	438	GLU	2.6
1	F	399	GLU	2.6
1	E	24	TRP	2.6
1	F	280	PHE	2.6
1	E	260	TYR	2.6
1	B	48	PRO	2.5
1	E	23	VAL	2.5
1	E	217	ILE	2.5
1	F	48	PRO	2.5
1	E	293	LEU	2.5
1	E	36	ASP	2.5
1	E	33	ILE	2.4
1	E	422	THR	2.4
1	E	48	PRO	2.4
1	A	250	PHE	2.4
1	A	459	TYR	2.4
1	E	158	GLN	2.4
1	F	439	PRO	2.4
1	A	303	ILE	2.3
1	E	344	LEU	2.3
1	E	345	VAL	2.3
1	E	384	PHE	2.3
1	E	135	ASP	2.3
1	F	296	ILE	2.3
1	A	426	ASN	2.3
1	E	402	LEU	2.2
1	E	457	LEU	2.2
1	E	381	VAL	2.2
1	E	223	GLU	2.2
1	E	202	PHE	2.2
1	B	395	TYR	2.2
1	E	352	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	229	LEU	2.1
1	E	416	LEU	2.1
1	E	382	GLY	2.1
1	E	399	GLU	2.1
1	E	257	PHE	2.1
1	A	362	ASP	2.1
1	A	110	THR	2.1
1	B	462	GLY	2.1
1	B	475	VAL	2.0
1	F	468	ALA	2.0
1	E	109	GLY	2.0
1	E	57	PRO	2.0
1	F	355	LEU	2.0
1	A	348	ASN	2.0
1	E	359	ALA	2.0
1	E	412	PHE	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 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
4	SO4	B	502	5/5	0.71	0.07	174,175,175,175	0
4	SO4	B	501	5/5	0.90	0.09	154,156,157,158	0

6.5 Other polymers [i](#)

There are no such residues in this entry.