



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:14 PM UTC

PDB ID : 1NOZ / pdb_00001noz
Title : T4 DNA POLYMERASE FRAGMENT (RESIDUES 1-388) AT 110K
Authors : Wang, J.; Yu, P.; Lin, T.C.; Konigsberg, W.H.; Steitz, T.A.
Deposited on : 1996-02-16
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

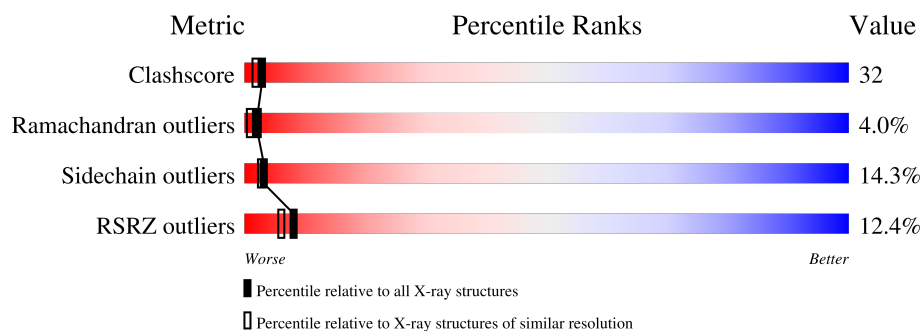
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	388	9% 40% 37% 10% • 11%
1	B	388	14% 30% 41% 15% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5725 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 POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2840	1822	466	533	19			
1	B	346	Total	C	N	O	S	0	0	0
			2840	1822	466	533	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	LYS	conflict	UNP P04415
A	250	LEU	ILE	conflict	UNP P04415
B	2	ASP	LYS	conflict	UNP P04415
B	250	LEU	ILE	conflict	UNP P04415

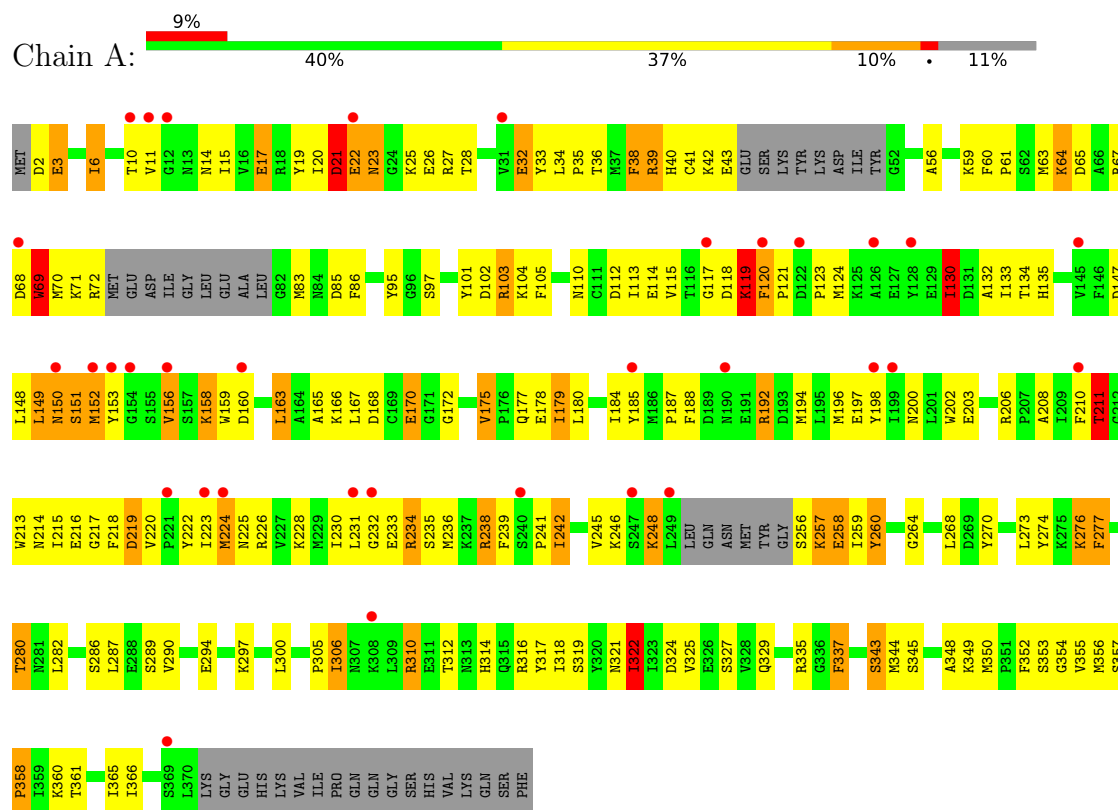
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total	O	0	0
			34	34		
2	B	11	Total	O	0	0
			11	11		

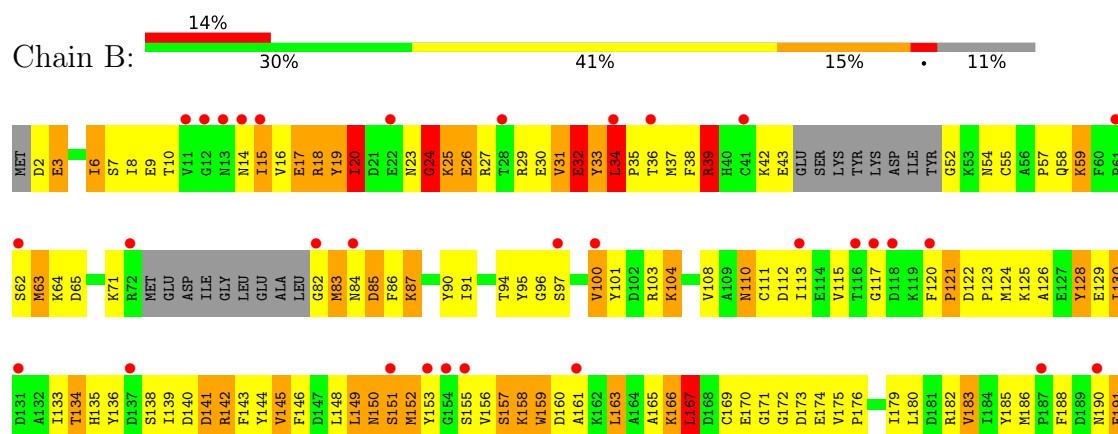
3 Residue-property plots

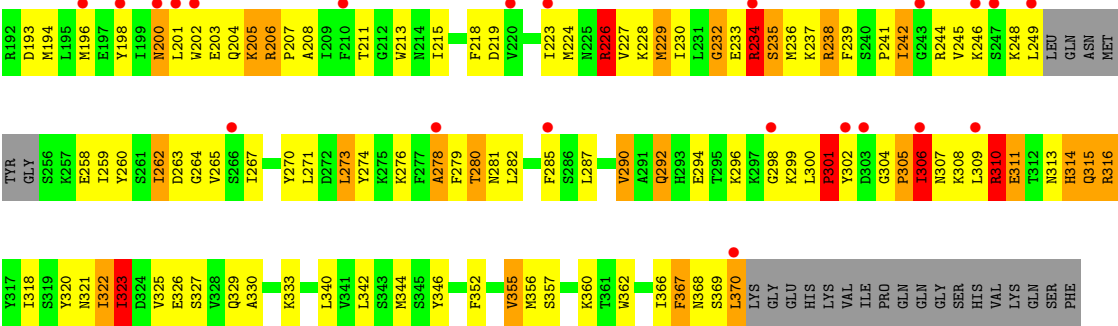
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: DNA POLYMERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	113.62Å 109.31Å 68.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20 6.00 – 2.72	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.20) 72.2 (6.00-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.67 (at 2.73Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.222 , (Not available) 0.315 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 152.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	5725	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.09% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.80	2/2904 (0.1%)	1.23	23/3911 (0.6%)
1	B	0.74	1/2904 (0.0%)	1.33	45/3911 (1.2%)
All	All	0.77	3/5808 (0.1%)	1.28	68/7822 (0.9%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	262	ILE	CA-CB	6.40	1.61	1.53
1	A	224	MET	SD-CE	-5.08	1.66	1.79
1	A	322	ILE	CA-CB	5.05	1.61	1.54

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	ILE	N-CA-C	-10.50	101.61	111.48
1	B	85	ASP	N-CA-C	-9.73	98.02	112.04
1	A	32	GLU	N-CA-C	-8.80	94.39	108.73
1	B	183	VAL	N-CA-C	8.69	119.72	107.37
1	B	235	SER	N-CA-C	-8.68	101.01	111.69
1	A	177	GLN	N-CA-C	8.60	120.73	111.36
1	A	335	ARG	N-CA-C	8.37	122.77	112.23
1	B	158	LYS	N-CA-C	-8.27	99.94	110.19
1	B	166	LYS	N-CA-C	8.23	122.14	108.73
1	A	175	VAL	N-CA-C	-7.99	101.76	108.63
1	B	208	ALA	N-CA-C	-7.97	102.53	111.14
1	B	280	THR	N-CA-C	7.87	127.56	110.80
1	B	96	GLY	N-CA-C	-7.64	100.82	112.89
1	A	280	THR	N-CA-C	7.46	122.36	111.02
1	B	17	GLU	N-CA-C	7.41	120.49	108.41
1	A	38	PHE	N-CA-C	7.35	126.46	110.80
1	B	242	ILE	N-CA-C	-7.33	105.26	111.56
1	A	179	ILE	N-CA-C	-7.31	103.73	110.82
1	B	310	ARG	N-CA-C	-7.22	103.35	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	ASP	N-CA-C	-7.21	97.98	109.59
1	B	32	GLU	N-CA-C	-7.06	98.45	109.25
1	B	316	ARG	N-CA-C	-7.05	103.60	111.28
1	A	69	TRP	N-CA-C	-6.75	103.17	111.40
1	B	24	GLY	N-CA-C	6.73	129.13	113.18
1	B	84	ASN	N-CA-C	-6.71	105.49	113.21
1	A	208	ALA	N-CA-C	-6.64	103.97	111.14
1	B	20	ILE	N-CA-C	-6.61	98.91	108.36
1	B	314	HIS	N-CA-C	-6.61	99.48	109.60
1	B	155	SER	N-CA-C	-6.40	99.20	109.96
1	A	211	THR	CB-CA-C	-6.33	103.18	113.37
1	B	128	TYR	N-CA-C	6.31	118.86	110.53
1	A	242	ILE	N-CA-C	-6.17	106.70	113.43
1	B	149	LEU	N-CA-C	-6.14	99.64	109.96
1	A	257	LYS	N-CA-C	6.12	123.85	110.80
1	A	152	MET	N-CA-C	6.11	123.81	110.80
1	B	232	GLY	N-CA-C	6.10	119.12	112.29
1	B	31	VAL	N-CA-C	6.09	118.15	108.89
1	B	38	PHE	N-CA-C	5.98	123.53	110.80
1	B	264	GLY	N-CA-C	-5.93	107.42	114.48
1	A	219	ASP	N-CA-C	5.92	118.24	111.02
1	B	145	VAL	N-CA-C	5.89	116.08	107.37
1	B	167	LEU	N-CA-C	5.84	123.24	110.80
1	A	258	GLU	N-CA-C	-5.83	98.38	110.80
1	A	277	PHE	N-CA-C	5.80	121.26	113.72
1	B	34	LEU	CA-C-N	5.76	126.67	119.98
1	B	34	LEU	C-N-CA	5.76	126.67	119.98
1	A	134	THR	N-CA-C	-5.69	100.42	109.76
1	A	203	GLU	N-CA-C	5.65	117.43	111.28
1	A	264	GLY	N-CA-C	-5.59	107.33	114.37
1	A	130	ILE	N-CA-C	-5.57	102.39	109.58
1	A	310	ARG	N-CA-C	-5.55	105.31	111.36
1	B	33	TYR	N-CA-C	5.47	118.38	109.24
1	B	304	GLY	CA-C-N	5.47	126.68	119.84
1	B	304	GLY	C-N-CA	5.47	126.68	119.84
1	B	246	LYS	N-CA-C	5.45	118.46	109.85
1	B	290	VAL	N-CA-C	5.45	115.89	110.23
1	B	134	THR	N-CA-C	-5.38	100.42	109.07
1	B	226	ARG	N-CA-C	-5.32	105.40	111.14
1	A	343	SER	N-CA-C	-5.25	105.25	110.97
1	A	337	PHE	N-CA-C	5.14	116.96	111.36
1	B	100	VAL	N-CA-C	-5.12	100.94	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	TRP	N-CA-C	-5.12	101.53	109.72
1	B	323	ILE	N-CA-C	5.11	115.32	110.42
1	B	294	GLU	N-CA-C	5.07	116.61	111.14
1	B	19	TYR	N-CA-C	5.06	115.99	108.60
1	B	368	ASN	N-CA-C	5.06	118.55	112.38
1	B	229	MET	N-CA-C	5.04	116.46	111.07
1	B	278	ALA	N-CA-C	-5.00	102.67	110.42

There are no chirality outliers.

There are no planarity outliers.

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	2840	0	2783	158	0
1	B	2840	0	2783	217	0
2	A	34	0	0	2	0
2	B	11	0	0	1	0
All	All	5725	0	5566	364	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 32.

All (364) 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:B:169:CYS:SG	1:B:170:GLU:HG3	2.05	0.97
1:A:114:GLU:HB2	1:A:132:ALA:HB3	1.53	0.88
1:B:179:ILE:HG22	1:B:322:ILE:HD11	1.62	0.82
1:A:224:MET:HE1	1:A:239:PHE:CD2	2.15	0.81
1:A:67:ARG:O	1:A:71:LYS:HG2	1.81	0.81
1:B:10:THR:HG23	1:B:14:ASN:O	1.81	0.79
1:B:19:TYR:CE1	1:B:29:ARG:HG3	2.17	0.79
1:A:160:ASP:OD2	1:A:163:LEU:HB2	1.82	0.79
1:B:17:GLU:OE1	1:B:29:ARG:HD2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:LEU:O	1:B:150:ASN:HB2	1.85	0.77
1:A:130:ILE:HD11	1:A:133:ILE:HG12	1.69	0.75
1:B:57:PRO:HG2	1:B:370:LEU:CD2	2.17	0.75
1:A:102:ASP:HB3	1:A:105:PHE:HD2	1.52	0.74
1:B:159:TRP:HD1	1:B:315:GLN:HA	1.52	0.74
1:B:113:ILE:HD11	1:B:218:PHE:CE2	2.23	0.74
1:B:224:MET:HE3	1:B:262:ILE:HD11	1.70	0.74
1:A:224:MET:HE2	1:A:245:VAL:HG11	1.70	0.73
1:A:130:ILE:HD11	1:A:133:ILE:CG1	2.19	0.73
1:A:158:LYS:HE2	1:A:185:TYR:CE2	2.23	0.73
1:B:143:PHE:HE1	1:B:182:ARG:HE	1.37	0.73
1:B:20:ILE:HG23	1:B:24:GLY:HA2	1.72	0.72
1:B:25:LYS:HA	1:B:25:LYS:HE2	1.72	0.72
1:A:230:ILE:HG22	1:A:231:LEU:HD22	1.72	0.71
1:B:156:VAL:HG11	1:B:314:HIS:CD2	2.25	0.70
1:B:110:ASN:HB2	1:B:211:THR:HG23	1.74	0.70
1:A:2:ASP:O	1:A:3:GLU:HB2	1.91	0.70
1:A:36:THR:HG22	1:A:59:LYS:HG3	1.74	0.69
1:B:144:TYR:HD2	1:B:186:MET:HE1	1.57	0.69
1:B:90:TYR:CZ	1:B:94:THR:HG21	2.28	0.69
1:B:163:LEU:HD11	1:B:171:GLY:O	1.94	0.68
1:B:249:LEU:HB3	1:B:258:GLU:HB3	1.75	0.68
1:B:39:ARG:HH12	1:B:42:LYS:NZ	1.92	0.68
1:B:241:PRO:HD2	1:B:263:ASP:O	1.94	0.68
1:B:344:MET:HE2	1:B:355:VAL:HB	1.75	0.67
1:A:158:LYS:HE2	1:A:185:TYR:HE2	1.56	0.67
1:A:273:LEU:HD12	1:A:356:MET:HE1	1.77	0.67
1:A:228:LYS:O	1:A:232:GLY:HA2	1.95	0.67
1:B:141:ASP:O	1:B:182:ARG:HG2	1.95	0.66
1:A:56:ALA:HB2	1:B:340:LEU:HD22	1.78	0.66
1:B:156:VAL:HG22	1:B:157:SER:H	1.61	0.66
1:A:179:ILE:HG22	1:A:322:ILE:HD11	1.77	0.65
1:B:179:ILE:CG2	1:B:322:ILE:HD11	2.27	0.64
1:A:213:TRP:HZ2	1:A:290:VAL:HG21	1.63	0.64
1:A:248:LYS:O	1:A:258:GLU:HA	1.97	0.64
1:A:196:MET:HG3	1:A:231:LEU:HD11	1.78	0.64
1:A:23:ASN:ND2	1:A:25:LYS:HG3	2.13	0.63
1:A:348:ALA:HB3	1:A:350:MET:HG2	1.81	0.63
1:B:151:SER:O	1:B:153:TYR:N	2.31	0.63
1:A:11:VAL:O	1:A:14:ASN:HB2	1.98	0.63
1:B:166:LYS:O	1:B:172:GLY:HA3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:HA	1:A:156:VAL:HG12	1.82	0.61
1:A:310:ARG:HD2	2:A:392:HOH:O	1.98	0.61
1:B:299:LYS:HE2	1:B:323:ILE:CG2	2.29	0.61
1:A:211:THR:HG21	1:A:270:TYR:HD2	1.64	0.61
1:B:248:LYS:O	1:B:258:GLU:HA	1.99	0.61
1:B:282:LEU:HB2	1:B:285:PHE:CE1	2.36	0.61
1:B:83:MET:SD	1:B:86:PHE:HB2	2.39	0.61
1:B:121:PRO:O	1:B:218:PHE:HE1	1.84	0.61
1:B:122:ASP:OD2	1:B:124:MET:HB2	2.01	0.61
1:B:179:ILE:HG22	1:B:322:ILE:CD1	2.30	0.60
1:A:224:MET:HE3	1:A:236:MET:HG3	1.81	0.60
1:B:83:MET:C	1:B:85:ASP:H	2.07	0.60
1:B:19:TYR:HE1	1:B:29:ARG:HG3	1.63	0.60
1:A:110:ASN:ND2	1:A:329:GLN:HE21	1.98	0.60
1:B:103:ARG:HG3	1:B:103:ARG:HH11	1.64	0.60
1:B:33:TYR:CD2	1:B:86:PHE:CE1	2.90	0.59
1:A:61:PRO:HD2	1:A:65:ASP:OD2	2.03	0.59
1:A:121:PRO:O	1:A:218:PHE:HE1	1.85	0.59
1:B:8:ILE:HD13	1:B:17:GLU:HG3	1.85	0.59
1:A:124:MET:SD	1:A:256:SER:O	2.61	0.59
1:A:213:TRP:CZ2	1:A:290:VAL:HG21	2.38	0.59
1:A:246:LYS:O	1:A:260:TYR:HA	2.03	0.59
1:A:39:ARG:HB3	1:A:42:LYS:HG2	1.85	0.59
1:B:130:ILE:HD11	1:B:133:ILE:HG13	1.85	0.59
1:A:306:ILE:HD12	1:A:306:ILE:H	1.68	0.58
1:B:33:TYR:HD2	1:B:86:PHE:CE1	2.21	0.58
1:B:124:MET:SD	1:B:258:GLU:HG2	2.42	0.58
1:B:2:ASP:O	1:B:3:GLU:HB3	2.03	0.58
1:A:228:LYS:HG3	1:A:233:GLU:HG3	1.85	0.58
1:B:203:GLU:OE2	1:B:238:ARG:HD2	2.04	0.58
1:A:318:ILE:O	1:A:322:ILE:HG23	2.04	0.58
1:A:83:MET:O	1:A:86:PHE:HB3	2.04	0.58
1:B:85:ASP:CG	1:B:367:PHE:HZ	2.12	0.58
1:B:37:MET:SD	1:B:370:LEU:HB3	2.44	0.57
1:B:306:ILE:HG22	1:B:307:ASN:N	2.19	0.57
1:A:345:SER:OG	1:A:352:PHE:HA	2.03	0.57
1:B:135:HIS:HD2	1:B:198:TYR:OH	1.88	0.57
1:B:15:ILE:HG21	1:B:90:TYR:CD2	2.40	0.57
1:B:156:VAL:HB	1:B:310:ARG:NH2	2.20	0.57
1:A:344:MET:SD	1:B:366:ILE:HG12	2.45	0.57
1:B:143:PHE:HE1	1:B:182:ARG:NE	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ILE:HD11	1:B:218:PHE:HE2	1.68	0.56
1:B:302:TYR:HE1	1:B:309:LEU:HD22	1.71	0.56
1:A:38:PHE:HD2	1:A:69:TRP:CZ3	2.24	0.56
1:B:19:TYR:O	1:B:26:GLU:HA	2.06	0.56
1:A:33:TYR:HD2	1:A:86:PHE:CE1	2.24	0.56
1:A:214:ASN:HD21	1:A:217:GLY:HA3	1.69	0.56
1:A:286:SER:O	1:A:290:VAL:HG23	2.06	0.56
1:A:358:PRO:HA	1:B:362:TRP:HB2	1.86	0.56
1:B:235:SER:O	1:B:238:ARG:HB2	2.06	0.56
1:B:309:LEU:HD11	1:B:313:ASN:HB3	1.87	0.56
1:A:149:LEU:HD11	1:A:187:PRO:HB2	1.87	0.56
1:B:16:VAL:HG12	1:B:30:GLU:HG3	1.86	0.56
1:B:326:GLU:HB3	2:B:394:HOH:O	2.06	0.56
1:B:37:MET:HG2	1:B:59:LYS:HA	1.88	0.56
1:B:308:LYS:HG3	1:B:311:GLU:HG3	1.87	0.56
1:A:6:ILE:HD13	1:A:20:ILE:HG12	1.87	0.55
1:A:43:GLU:HG2	1:A:69:TRP:CZ3	2.41	0.55
1:B:310:ARG:O	1:B:314:HIS:HB2	2.06	0.55
1:B:152:MET:SD	1:B:153:TYR:CD1	3.00	0.55
1:A:158:LYS:HB3	1:A:158:LYS:NZ	2.22	0.55
1:B:163:LEU:HD22	1:B:163:LEU:O	2.06	0.55
1:A:235:SER:HA	1:A:238:ARG:HG3	1.89	0.55
1:A:366:ILE:HG12	1:B:344:MET:SD	2.47	0.55
1:A:357:SER:OG	1:A:360:LYS:HB2	2.07	0.54
1:B:110:ASN:HA	1:B:211:THR:O	2.08	0.54
1:A:38:PHE:HB2	1:A:69:TRP:CH2	2.42	0.54
1:B:299:LYS:HE2	1:B:323:ILE:HG21	1.89	0.54
1:A:274:TYR:CE2	1:A:280:THR:HG21	2.42	0.54
1:B:226:ARG:NH2	1:B:229:MET:SD	2.80	0.54
1:B:57:PRO:HG2	1:B:370:LEU:HD23	1.90	0.54
1:B:270:TYR:HA	1:B:273:LEU:HG	1.90	0.54
1:A:63:MET:HG2	1:A:67:ARG:HH21	1.72	0.54
1:A:259:ILE:O	1:A:260:TYR:HB2	2.07	0.53
1:A:102:ASP:HB3	1:A:105:PHE:CD2	2.40	0.53
1:A:310:ARG:HG3	1:A:317:TYR:CD2	2.43	0.53
1:B:36:THR:O	1:B:59:LYS:HG3	2.09	0.53
1:B:64:LYS:HG3	1:B:65:ASP:N	2.23	0.53
1:B:145:VAL:CG2	1:B:183:VAL:HG13	2.39	0.53
1:B:308:LYS:CG	1:B:311:GLU:HB2	2.38	0.53
1:A:344:MET:HB3	1:A:355:VAL:HG22	1.91	0.53
1:A:34:LEU:CD2	1:A:70:MET:HG3	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLU:O	1:B:234:ARG:HB3	2.09	0.52
1:A:188:PHE:CD1	1:A:194:MET:HG3	2.43	0.52
1:B:302:TYR:OH	1:B:309:LEU:HD13	2.10	0.52
1:B:357:SER:HB3	1:B:360:LYS:HB2	1.89	0.52
1:A:135:HIS:HD2	1:A:198:TYR:OH	1.93	0.52
1:A:211:THR:HG23	1:A:268:LEU:O	2.10	0.52
1:B:213:TRP:NE1	1:B:271:LEU:HD13	2.25	0.52
1:A:36:THR:O	1:A:59:LYS:HG3	2.10	0.52
1:B:144:TYR:CD2	1:B:186:MET:HE1	2.42	0.52
1:A:166:LYS:O	1:A:172:GLY:HA3	2.10	0.52
1:B:201:LEU:O	1:B:205:LYS:HG3	2.10	0.52
1:A:69:TRP:HA	1:A:72:ARG:CZ	2.40	0.51
1:B:117:GLY:HA2	1:B:153:TYR:OH	2.10	0.51
1:A:117:GLY:HA2	1:A:153:TYR:CZ	2.44	0.51
1:A:156:VAL:HG11	1:A:314:HIS:CD2	2.45	0.51
1:B:8:ILE:CD1	1:B:17:GLU:HG3	2.41	0.51
1:B:103:ARG:HH12	1:B:108:VAL:HG21	1.76	0.51
1:A:206:ARG:NH2	1:A:238:ARG:O	2.44	0.51
1:A:113:ILE:HG22	1:A:133:ILE:HG12	1.91	0.51
1:B:64:LYS:HG3	1:B:65:ASP:H	1.75	0.51
1:A:179:ILE:HG22	1:A:322:ILE:CD1	2.40	0.51
1:B:113:ILE:HD12	1:B:115:VAL:HG23	1.93	0.51
1:B:200:ASN:O	1:B:204:GLN:HG3	2.11	0.51
1:A:233:GLU:O	1:A:234:ARG:CB	2.58	0.51
1:A:159:TRP:HB3	1:A:185:TYR:CE1	2.46	0.51
1:B:121:PRO:HB3	1:B:128:TYR:CD2	2.46	0.51
1:A:33:TYR:CD2	1:A:86:PHE:CE1	2.99	0.50
1:B:308:LYS:O	1:B:308:LYS:HG2	2.11	0.50
1:B:71:LYS:O	1:B:71:LYS:HG2	2.11	0.50
1:B:308:LYS:HG2	1:B:311:GLU:HB2	1.93	0.50
1:A:123:PRO:HG3	1:A:218:PHE:CD1	2.46	0.50
1:A:216:GLU:HA	2:A:420:HOH:O	2.10	0.50
1:B:313:ASN:C	1:B:314:HIS:O	2.52	0.50
1:A:38:PHE:HB3	1:A:60:PHE:CZ	2.47	0.50
1:A:358:PRO:HG3	1:B:362:TRP:CE3	2.46	0.50
1:B:245:VAL:HG12	1:B:260:TYR:CE2	2.46	0.50
1:A:32:GLU:H	1:A:32:GLU:CD	2.19	0.50
1:B:103:ARG:HG3	1:B:103:ARG:NH1	2.27	0.50
1:B:190:ASN:OD1	1:B:193:ASP:HB2	2.12	0.50
1:A:118:ASP:O	1:A:120:PHE:N	2.45	0.49
1:B:136:TYR:CE2	1:B:138:SER:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLN:NE2	1:B:298:GLY:HA2	2.27	0.49
1:B:19:TYR:CZ	1:B:27:ARG:HB2	2.46	0.49
1:A:115:VAL:HG22	1:A:130:ILE:HA	1.93	0.49
1:B:57:PRO:HG2	1:B:370:LEU:HD21	1.95	0.49
1:B:146:PHE:HB3	1:B:194:MET:CG	2.43	0.49
1:A:36:THR:O	1:A:59:LYS:HA	2.13	0.49
1:B:245:VAL:HG12	1:B:260:TYR:CD2	2.47	0.49
1:B:299:LYS:HE2	1:B:323:ILE:HG22	1.93	0.49
1:B:183:VAL:HG21	1:B:322:ILE:HD13	1.93	0.49
1:A:34:LEU:HD23	1:A:70:MET:HG3	1.94	0.49
1:A:121:PRO:HB2	1:A:218:PHE:CE1	2.47	0.49
1:B:236:MET:O	1:B:239:PHE:HB2	2.13	0.49
1:B:215:ILE:HA	1:B:219:ASP:HB2	1.95	0.48
1:A:219:ASP:O	1:A:223:ILE:HG13	2.13	0.48
1:B:134:THR:HA	1:B:144:TYR:O	2.13	0.48
1:A:321:ASN:O	1:A:325:VAL:HG23	2.13	0.48
1:B:226:ARG:HE	1:B:226:ARG:HA	1.78	0.48
1:A:23:ASN:HD21	1:A:25:LYS:HG3	1.76	0.48
1:B:140:ASP:O	1:B:142:ARG:N	2.46	0.48
1:B:152:MET:SD	1:B:153:TYR:N	2.87	0.48
1:A:350:MET:HE2	1:A:354:GLY:HA3	1.96	0.48
1:B:153:TYR:HD1	1:B:153:TYR:H	1.62	0.48
1:A:17:GLU:O	1:A:28:THR:HA	2.14	0.47
1:B:10:THR:O	1:B:244:ARG:NH2	2.47	0.47
1:B:175:VAL:HG22	1:B:323:ILE:HD11	1.96	0.47
1:A:167:LEU:O	1:A:170:GLU:HG2	2.13	0.47
1:A:147:ASP:O	1:A:187:PRO:HA	2.14	0.47
1:B:165:ALA:HB2	1:B:180:LEU:CD1	2.44	0.47
1:A:38:PHE:CD2	1:A:69:TRP:CZ3	3.03	0.47
1:A:70:MET:HE2	1:A:70:MET:HA	1.96	0.47
1:A:192:ARG:HB2	1:A:192:ARG:NH1	2.30	0.47
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.71	0.47
1:A:102:ASP:OD2	1:A:104:LYS:HE2	2.15	0.47
1:A:119:LYS:O	1:A:120:PHE:CB	2.63	0.47
1:B:34:LEU:HA	1:B:35:PRO:HD3	1.75	0.47
1:B:129:GLU:HA	1:B:191:GLU:OE2	2.15	0.47
1:B:156:VAL:HG22	1:B:157:SER:N	2.29	0.47
1:B:292:GLN:O	1:B:296:LYS:HA	2.15	0.47
1:A:276:LYS:NZ	1:A:356:MET:SD	2.80	0.46
1:B:121:PRO:HB3	1:B:128:TYR:HD2	1.81	0.46
1:B:145:VAL:HG23	1:B:183:VAL:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ARG:NH2	1:B:238:ARG:O	2.47	0.46
1:A:35:PRO:HD3	1:A:86:PHE:CE1	2.51	0.46
1:A:119:LYS:O	1:A:120:PHE:HB2	2.15	0.46
1:A:175:VAL:CG2	1:A:319:SER:HB3	2.45	0.46
1:B:176:PRO:HD2	1:B:179:ILE:HD12	1.97	0.46
1:B:213:TRP:CZ2	1:B:290:VAL:HG21	2.50	0.46
1:A:10:THR:HA	1:A:14:ASN:O	2.16	0.46
1:B:159:TRP:CH2	1:B:161:ALA:HA	2.51	0.46
1:B:280:THR:OG1	1:B:285:PHE:HZ	1.98	0.46
1:A:10:THR:CG2	1:A:15:ILE:HD13	2.44	0.46
1:B:34:LEU:HD11	1:B:63:MET:HG2	1.98	0.46
1:A:297:LYS:HE2	1:A:297:LYS:HA	1.98	0.46
1:B:203:GLU:CD	1:B:238:ARG:HH11	2.24	0.46
1:B:309:LEU:CD1	1:B:313:ASN:HB3	2.45	0.46
1:A:228:LYS:O	1:A:232:GLY:CA	2.62	0.46
1:B:126:ALA:O	1:B:226:ARG:NH2	2.48	0.46
1:A:166:LYS:C	1:A:172:GLY:HA3	2.41	0.46
1:B:175:VAL:HG22	1:B:323:ILE:CD1	2.45	0.46
1:A:20:ILE:HG13	1:A:105:PHE:HB3	1.98	0.45
1:A:61:PRO:HD2	1:A:65:ASP:CG	2.42	0.45
1:A:123:PRO:HA	1:A:222:TYR:CD2	2.52	0.45
1:A:361:THR:O	1:A:365:ILE:HG12	2.15	0.45
1:B:82:GLY:O	1:B:85:ASP:HB2	2.17	0.45
1:B:113:ILE:HG22	1:B:133:ILE:HG12	1.98	0.45
1:B:207:PRO:O	1:B:265:VAL:HG13	2.17	0.45
1:A:206:ARG:HD3	1:A:241:PRO:HD3	1.98	0.45
1:A:213:TRP:CH2	1:A:290:VAL:HG11	2.51	0.45
1:B:101:TYR:CD1	1:B:101:TYR:N	2.84	0.45
1:B:300:LEU:HD12	1:B:301:PRO:HD2	1.99	0.45
1:B:62:SER:O	1:B:64:LYS:N	2.49	0.45
1:A:119:LYS:HA	1:A:119:LYS:HD2	1.76	0.45
1:B:112:ASP:HB2	1:B:325:VAL:CG2	2.47	0.45
1:B:120:PHE:O	1:B:122:ASP:N	2.49	0.45
1:B:233:GLU:O	1:B:234:ARG:CB	2.64	0.45
1:B:314:HIS:O	1:B:316:ARG:N	2.50	0.45
1:B:134:THR:N	1:B:321:ASN:HD21	2.13	0.45
1:B:31:VAL:HG12	1:B:32:GLU:O	2.17	0.45
1:B:123:PRO:HG3	1:B:218:PHE:CD1	2.52	0.45
1:B:148:LEU:HB2	1:B:194:MET:HE1	1.99	0.45
1:B:163:LEU:HD21	1:B:171:GLY:C	2.42	0.45
1:A:10:THR:HG22	1:A:15:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:HG3	1:B:3:GLU:O	2.15	0.44
1:B:83:MET:C	1:B:85:ASP:N	2.75	0.44
1:A:358:PRO:HA	1:B:362:TRP:CG	2.51	0.44
1:B:149:LEU:O	1:B:150:ASN:CB	2.61	0.44
1:B:305:PRO:O	1:B:306:ILE:HG12	2.17	0.44
1:A:192:ARG:HB2	1:A:192:ARG:HH11	1.82	0.44
1:A:149:LEU:O	1:A:150:ASN:CG	2.60	0.44
1:B:42:LYS:HG2	1:B:85:ASP:OD1	2.17	0.44
1:B:146:PHE:CD1	1:B:146:PHE:N	2.86	0.44
1:A:32:GLU:CD	1:A:32:GLU:N	2.76	0.44
1:B:167:LEU:HB2	1:B:169:CYS:SG	2.58	0.44
1:A:36:THR:HG22	1:A:36:THR:O	2.18	0.44
1:B:87:LYS:O	1:B:91:ILE:HG13	2.18	0.44
1:B:167:LEU:CB	1:B:169:CYS:SG	3.06	0.44
1:B:327:SER:O	1:B:330:ALA:HB3	2.18	0.44
1:A:156:VAL:HG21	1:A:314:HIS:HB2	2.00	0.44
1:B:90:TYR:CE2	1:B:94:THR:HG21	2.53	0.43
1:B:91:ILE:O	1:B:95:TYR:HB2	2.18	0.43
1:A:165:ALA:HB2	1:A:180:LEU:CD1	2.47	0.43
1:A:225:ASN:ND2	1:A:260:TYR:OH	2.51	0.43
1:A:274:TYR:HE2	1:A:280:THR:HG21	1.83	0.43
1:B:62:SER:HB3	1:B:64:LYS:HG2	2.00	0.43
1:B:143:PHE:HZ	1:B:182:ARG:HH21	1.65	0.43
1:B:163:LEU:HD22	1:B:172:GLY:CA	2.48	0.43
1:A:95:TYR:O	1:A:349:LYS:NZ	2.47	0.43
1:A:149:LEU:HB3	1:A:156:VAL:HG12	2.01	0.43
1:B:7:SER:HB3	1:B:18:ARG:HB2	1.99	0.43
1:B:120:PHE:N	1:B:121:PRO:CD	2.82	0.43
1:B:262:ILE:HD13	1:B:267:ILE:HD11	2.01	0.43
1:B:342:LEU:O	1:B:346:TYR:CD2	2.71	0.43
1:B:200:ASN:ND2	1:B:204:GLN:OE1	2.51	0.43
1:A:149:LEU:CD2	1:A:158:LYS:HA	2.49	0.43
1:A:184:ILE:HG22	1:A:184:ILE:O	2.17	0.43
1:B:85:ASP:CG	1:B:367:PHE:CZ	2.94	0.43
1:B:140:ASP:O	1:B:142:ARG:CD	2.66	0.43
1:B:249:LEU:N	1:B:249:LEU:HD23	2.34	0.43
1:B:228:LYS:O	1:B:232:GLY:N	2.51	0.43
1:B:159:TRP:CD1	1:B:318:ILE:HB	2.54	0.42
1:B:356:MET:HE3	1:B:356:MET:HB3	1.89	0.42
1:B:169:CYS:SG	1:B:170:GLU:N	2.92	0.42
1:A:19:TYR:O	1:A:26:GLU:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:TYR:O	1:B:278:ALA:HB3	2.19	0.42
1:B:329:GLN:O	1:B:333:LYS:HG3	2.20	0.42
1:A:22:GLU:H	1:A:22:GLU:HG3	1.54	0.42
1:A:202:TRP:HZ2	1:A:210:PHE:CZ	2.37	0.42
1:B:196:MET:HE3	1:B:196:MET:HB3	1.86	0.42
1:B:232:GLY:O	1:B:235:SER:HB2	2.20	0.42
1:A:197:GLU:O	1:A:200:ASN:HB2	2.20	0.42
1:A:220:VAL:O	1:A:224:MET:HG2	2.20	0.42
1:B:305:PRO:HG2	1:B:306:ILE:H	1.84	0.42
1:A:41:CYS:HB3	1:B:279:PHE:CG	2.54	0.42
1:A:147:ASP:OD2	1:A:314:HIS:CE1	2.72	0.42
1:A:343:SER:HB2	1:B:369:SER:HB2	2.01	0.42
1:A:358:PRO:HA	1:B:362:TRP:CB	2.49	0.42
1:B:292:GLN:O	1:B:296:LYS:N	2.52	0.42
1:A:10:THR:HG21	1:A:86:PHE:CD2	2.55	0.42
1:A:270:TYR:OH	1:A:337:PHE:HB2	2.19	0.42
1:B:196:MET:CE	1:B:238:ARG:NH2	2.82	0.42
1:B:9:GLU:CG	1:B:10:THR:H	2.32	0.42
1:B:54:ASN:CG	1:B:55:CYS:H	2.28	0.42
1:B:117:GLY:HA3	1:B:128:TYR:CD2	2.54	0.42
1:B:134:THR:OG1	1:B:321:ASN:ND2	2.50	0.42
1:B:211:THR:C	1:B:215:ILE:HD13	2.44	0.42
1:A:166:LYS:HB3	1:A:170:GLU:HG3	2.01	0.42
1:B:115:VAL:HG22	1:B:130:ILE:HA	2.02	0.42
1:A:112:ASP:CB	1:A:325:VAL:HG22	2.50	0.41
1:B:104:LYS:N	1:B:104:LYS:HD2	2.34	0.41
1:B:196:MET:HE1	1:B:238:ARG:NH2	2.35	0.41
1:A:101:TYR:CD1	1:A:101:TYR:N	2.88	0.41
1:B:39:ARG:HH12	1:B:42:LYS:HZ3	1.67	0.41
1:B:103:ARG:NH1	1:B:103:ARG:CG	2.82	0.41
1:B:273:LEU:HD23	1:B:273:LEU:N	2.35	0.41
1:B:130:ILE:CD1	1:B:133:ILE:HG13	2.49	0.41
1:A:38:PHE:HB2	1:A:69:TRP:CZ2	2.55	0.41
1:A:42:LYS:HG3	1:A:85:ASP:OD2	2.21	0.41
1:A:168:ASP:HB2	1:A:300:LEU:HD13	2.03	0.41
1:A:112:ASP:HB2	1:A:325:VAL:HG22	2.02	0.41
1:B:227:VAL:O	1:B:232:GLY:N	2.53	0.41
1:B:202:TRP:CD1	1:B:239:PHE:HE1	2.38	0.41
1:A:21:ASP:OD2	1:A:22:GLU:N	2.54	0.41
1:A:135:HIS:CD2	1:A:198:TYR:OH	2.71	0.41
1:B:2:ASP:O	1:B:3:GLU:CB	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:PHE:CD1	1:B:194:MET:HG3	2.56	0.41
1:A:277:PHE:O	1:B:55:CYS:HA	2.21	0.41
1:A:324:ASP:O	1:A:327:SER:HB2	2.20	0.41
1:B:16:VAL:HA	1:B:29:ARG:O	2.21	0.41
1:B:198:TYR:HE2	1:B:223:ILE:HD13	1.85	0.41
1:B:299:LYS:HG3	1:B:300:LEU:N	2.34	0.41
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.96	0.41
1:B:320:TYR:O	1:B:323:ILE:HB	2.21	0.41
1:A:43:GLU:OE2	1:A:72:ARG:NH1	2.54	0.41
1:A:113:ILE:HG21	1:A:223:ILE:HD11	2.02	0.41
1:A:148:LEU:HB2	1:A:194:MET:SD	2.61	0.41
1:B:308:LYS:CG	1:B:308:LYS:O	2.68	0.41
1:B:159:TRP:HB3	1:B:185:TYR:CE1	2.56	0.40
1:B:234:ARG:HA	1:B:237:LYS:HB2	2.02	0.40
1:A:103:ARG:O	1:A:103:ARG:HG3	2.20	0.40
1:A:196:MET:O	1:A:200:ASN:ND2	2.52	0.40
1:A:357:SER:HA	1:A:358:PRO:HD3	1.98	0.40
1:B:35:PRO:HG3	1:B:86:PHE:HD1	1.85	0.40
1:B:145:VAL:HG21	1:B:183:VAL:HG13	2.03	0.40
1:A:64:LYS:HD3	1:A:68:ASP:OD2	2.21	0.40
1:B:18:ARG:NH1	1:B:26:GLU:OE2	2.54	0.40
1:B:167:LEU:HA	1:B:174:GLU:CG	2.52	0.40
1:B:201:LEU:HD11	1:B:205:LYS:HD2	2.04	0.40
1:B:352:PHE:O	1:B:355:VAL:HG13	2.21	0.40
1:A:40:HIS:O	1:A:43:GLU:HG3	2.22	0.40
1:A:276:LYS:HG2	1:B:52:GLY:O	2.21	0.40
1:B:151:SER:O	1:B:152:MET:C	2.64	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	338/388 (87%)	299 (88%)	27 (8%)	12 (4%)	2	1
1	B	338/388 (87%)	294 (87%)	29 (9%)	15 (4%)	2	1
All	All	676/776 (87%)	593 (88%)	56 (8%)	27 (4%)	2	1

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	PHE
1	A	150	ASN
1	A	257	LYS
1	B	3	GLU
1	B	141	ASP
1	B	152	MET
1	B	167	LEU
1	B	305	PRO
1	B	306	ILE
1	A	3	GLU
1	A	119	LYS
1	A	234	ARG
1	B	24	GLY
1	B	234	ARG
1	B	281	ASN
1	A	21	ASP
1	A	151	SER
1	A	152	MET
1	B	63	MET
1	A	260	TYR
1	B	121	PRO
1	A	39	ARG
1	A	305	PRO
1	B	39	ARG
1	B	150	ASN
1	B	104	LYS
1	B	301	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	312/350 (89%)	275 (88%)	37 (12%)	5	4
1	B	312/350 (89%)	260 (83%)	52 (17%)	2	2
All	All	624/700 (89%)	535 (86%)	89 (14%)	3	3

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	17	GLU
1	A	21	ASP
1	A	22	GLU
1	A	23	ASN
1	A	27	ARG
1	A	64	LYS
1	A	69	TRP
1	A	97	SER
1	A	103	ARG
1	A	119	LYS
1	A	130	ILE
1	A	149	LEU
1	A	151	SER
1	A	156	VAL
1	A	158	LYS
1	A	163	LEU
1	A	170	GLU
1	A	178	GLU
1	A	192	ARG
1	A	211	THR
1	A	215	ILE
1	A	226	ARG
1	A	238	ARG
1	A	242	ILE
1	A	248	LYS
1	A	276	LYS
1	A	282	LEU
1	A	287	LEU
1	A	289	SER
1	A	294	GLU
1	A	306	ILE
1	A	312	THR
1	A	316	ARG

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Mol	Chain	Res	Type
1	A	322	ILE
1	A	353	SER
1	A	358	PRO
1	B	6	ILE
1	B	15	ILE
1	B	18	ARG
1	B	20	ILE
1	B	23	ASN
1	B	25	LYS
1	B	26	GLU
1	B	32	GLU
1	B	34	LEU
1	B	39	ARG
1	B	43	GLU
1	B	58	GLN
1	B	59	LYS
1	B	83	MET
1	B	87	LYS
1	B	97	SER
1	B	100	VAL
1	B	110	ASN
1	B	111	CYS
1	B	125	LYS
1	B	130	ILE
1	B	139	ILE
1	B	142	ARG
1	B	151	SER
1	B	157	SER
1	B	158	LYS
1	B	160	ASP
1	B	163	LEU
1	B	191	GLU
1	B	200	ASN
1	B	205	LYS
1	B	206	ARG
1	B	226	ARG
1	B	230	ILE
1	B	234	ARG
1	B	238	ARG
1	B	242	ILE
1	B	259	ILE
1	B	273	LEU

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Mol	Chain	Res	Type
1	B	276	LYS
1	B	287	LEU
1	B	292	GLN
1	B	301	PRO
1	B	306	ILE
1	B	310	ARG
1	B	311	GLU
1	B	315	GLN
1	B	322	ILE
1	B	323	ILE
1	B	355	VAL
1	B	367	PHE
1	B	370	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	23	ASN
1	A	58	GLN
1	A	110	ASN
1	A	135	HIS
1	A	150	ASN
1	A	177	GLN
1	A	190	ASN
1	A	214	ASN
1	A	225	ASN
1	A	313	ASN
1	A	329	GLN
1	A	368	ASN
1	B	135	HIS
1	B	150	ASN
1	B	200	ASN
1	B	204	GLN
1	B	313	ASN
1	B	315	GLN
1	B	321	ASN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	346/388 (89%)	0.81	33 (9%) 14 11	20, 39, 61, 72	0
1	B	346/388 (89%)	1.05	53 (15%) 5 4	25, 54, 87, 101	0
All	All	692/776 (89%)	0.93	86 (12%) 8 6	20, 46, 78, 101	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	118	ASP	4.9
1	A	12	GLY	4.8
1	A	154	GLY	4.5
1	B	198	TYR	4.4
1	B	82	GLY	4.2
1	B	243	GLY	4.0
1	B	210	PHE	3.7
1	B	116	THR	3.6
1	B	200	ASN	3.5
1	B	62	SER	3.3
1	B	309	LEU	3.3
1	A	120	PHE	3.3
1	B	12	GLY	3.2
1	A	122	ASP	3.1
1	B	190	ASN	3.1
1	B	196	MET	2.9
1	B	11	VAL	2.9
1	A	240	SER	2.9
1	A	152	MET	2.9
1	A	11	VAL	2.9
1	B	298	GLY	2.8
1	B	13	ASN	2.8
1	B	154	GLY	2.8
1	A	249	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	266	SER	2.7
1	A	150	ASN	2.7
1	A	126	ALA	2.7
1	B	302	TYR	2.7
1	B	120	PHE	2.7
1	B	223	ILE	2.6
1	B	201	LEU	2.6
1	B	161	ALA	2.6
1	B	84	ASN	2.6
1	A	231	LEU	2.6
1	B	202	TRP	2.6
1	A	22	GLU	2.5
1	B	234	ARG	2.5
1	B	97	SER	2.5
1	A	223	ILE	2.5
1	B	247	SER	2.5
1	B	153	TYR	2.4
1	B	61	PRO	2.4
1	A	198	TYR	2.4
1	B	15	ILE	2.4
1	B	187	PRO	2.3
1	B	151	SER	2.3
1	B	155	SER	2.3
1	B	113	ILE	2.3
1	B	285	PHE	2.3
1	B	137	ASP	2.3
1	A	128	TYR	2.3
1	A	224	MET	2.3
1	A	156	VAL	2.3
1	A	160	ASP	2.3
1	A	117	GLY	2.3
1	B	36	THR	2.3
1	A	247	SER	2.3
1	B	246	LYS	2.3
1	B	306	ILE	2.3
1	B	249	LEU	2.2
1	A	68	ASP	2.2
1	B	14	ASN	2.2
1	B	72	ARG	2.2
1	B	41	CYS	2.2
1	A	232	GLY	2.2
1	B	117	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	210	PHE	2.2
1	A	369	SER	2.2
1	B	34	LEU	2.1
1	B	220	VAL	2.1
1	B	22	GLU	2.1
1	A	153	TYR	2.1
1	A	31	VAL	2.1
1	A	221	PRO	2.1
1	A	10	THR	2.1
1	A	199	ILE	2.1
1	A	185	TYR	2.1
1	A	145	VAL	2.1
1	B	100	VAL	2.1
1	B	370	LEU	2.0
1	A	308	LYS	2.0
1	B	28	THR	2.0
1	B	278	ALA	2.0
1	A	190	ASN	2.0
1	B	131	ASP	2.0
1	B	303	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.