



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:26 PM UTC

PDB ID : 7S00 / pdb_00007s00
Title : X-ray structure of the phage AR9 non-virion RNA polymerase core
Authors : Leiman, P.G.; Sokolova, M.L.; Fraser, A.
Deposited on : 2021-08-28
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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

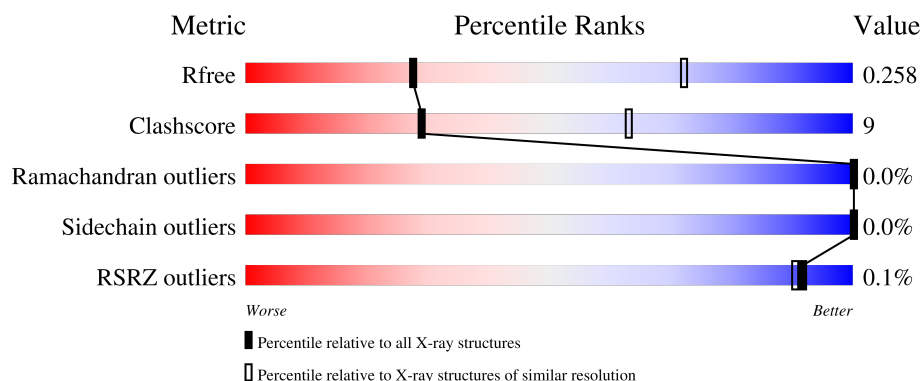
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

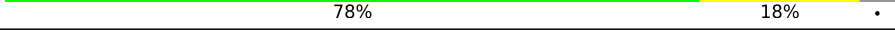
The reported resolution of this entry is 3.30 Å.

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	c	496	
1	e	496	
2	C	665	
2	E	665	
3	D	631	

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Mol	Chain	Length	Quality of chain
3	F	631	 74% 20% 6%
4	d	448	 67% 24% 8%
4	f	448	 75% 17% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33894 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-directed RNA polymerase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	484	Total	C	N	O	S	0	0	0
			4003	2580	658	754	11			
1	e	484	Total	C	N	O	S	0	0	0
			4003	2580	658	754	11			

- Molecule 2 is a protein called DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	640	Total	C	N	O	S	0	1	0
			5208	3296	857	1031	24			
2	E	640	Total	C	N	O	S	0	1	0
			5208	3296	857	1031	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	481	Total	C	N	O	S	0	0	0
			3893	2481	640	757	15			
3	F	596	Total	C	N	O	S	0	0	0
			4853	3092	791	952	18			

- Molecule 4 is a protein called DNA-directed RNA polymerase beta' subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	410	Total	C	N	O	S	0	0	0
			3362	2182	541	631	8			
4	f	410	Total	C	N	O	S	0	0	0
			3362	2182	541	631	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-21	MET	-	expression tag	UNP A0A172JIH0
d	-20	GLY	-	expression tag	UNP A0A172JIH0
d	-19	SER	-	expression tag	UNP A0A172JIH0
d	-18	SER	-	expression tag	UNP A0A172JIH0
d	-17	HIS	-	expression tag	UNP A0A172JIH0
d	-16	HIS	-	expression tag	UNP A0A172JIH0
d	-15	HIS	-	expression tag	UNP A0A172JIH0
d	-14	HIS	-	expression tag	UNP A0A172JIH0
d	-13	HIS	-	expression tag	UNP A0A172JIH0
d	-12	HIS	-	expression tag	UNP A0A172JIH0
d	-11	SER	-	expression tag	UNP A0A172JIH0
d	-10	SER	-	expression tag	UNP A0A172JIH0
d	-9	GLY	-	expression tag	UNP A0A172JIH0
d	-8	GLU	-	expression tag	UNP A0A172JIH0
d	-7	ASN	-	expression tag	UNP A0A172JIH0
d	-6	LEU	-	expression tag	UNP A0A172JIH0
d	-5	TYR	-	expression tag	UNP A0A172JIH0
d	-4	PHE	-	expression tag	UNP A0A172JIH0
d	-3	GLN	-	expression tag	UNP A0A172JIH0
d	-2	GLY	-	expression tag	UNP A0A172JIH0
d	-1	HIS	-	expression tag	UNP A0A172JIH0
d	0	HIS	-	expression tag	UNP A0A172JIH0
f	-21	MET	-	expression tag	UNP A0A172JIH0
f	-20	GLY	-	expression tag	UNP A0A172JIH0
f	-19	SER	-	expression tag	UNP A0A172JIH0
f	-18	SER	-	expression tag	UNP A0A172JIH0
f	-17	HIS	-	expression tag	UNP A0A172JIH0
f	-16	HIS	-	expression tag	UNP A0A172JIH0
f	-15	HIS	-	expression tag	UNP A0A172JIH0
f	-14	HIS	-	expression tag	UNP A0A172JIH0
f	-13	HIS	-	expression tag	UNP A0A172JIH0
f	-12	HIS	-	expression tag	UNP A0A172JIH0
f	-11	SER	-	expression tag	UNP A0A172JIH0
f	-10	SER	-	expression tag	UNP A0A172JIH0
f	-9	GLY	-	expression tag	UNP A0A172JIH0
f	-8	GLU	-	expression tag	UNP A0A172JIH0
f	-7	ASN	-	expression tag	UNP A0A172JIH0
f	-6	LEU	-	expression tag	UNP A0A172JIH0
f	-5	TYR	-	expression tag	UNP A0A172JIH0
f	-4	PHE	-	expression tag	UNP A0A172JIH0
f	-3	GLN	-	expression tag	UNP A0A172JIH0
f	-2	GLY	-	expression tag	UNP A0A172JIH0
f	-1	HIS	-	expression tag	UNP A0A172JIH0

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Chain	Residue	Modelled	Actual	Comment	Reference
f	0	HIS	-	expression tag	UNP A0A172JIH0

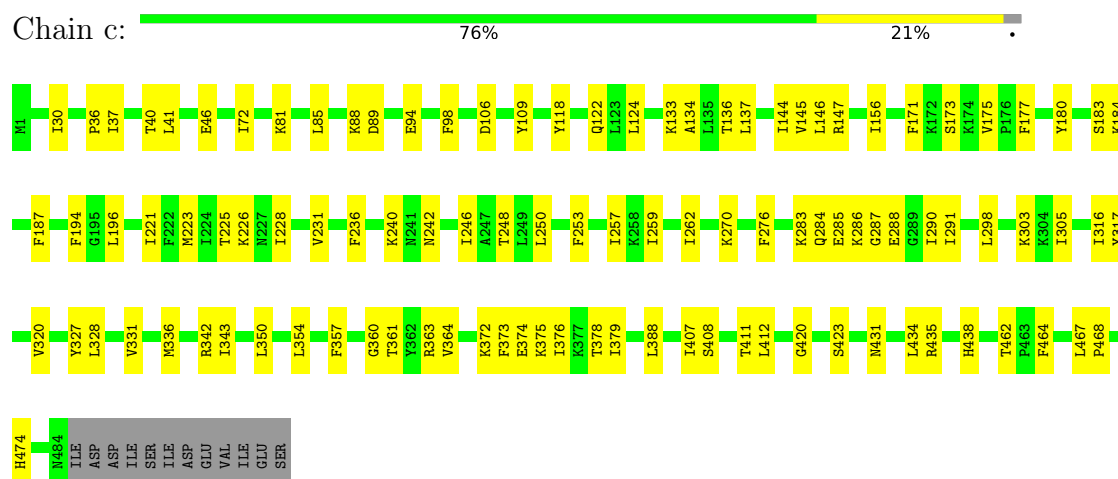
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Zn	0	0
			1	1		
5	F	1	Total	Zn	0	0
			1	1		

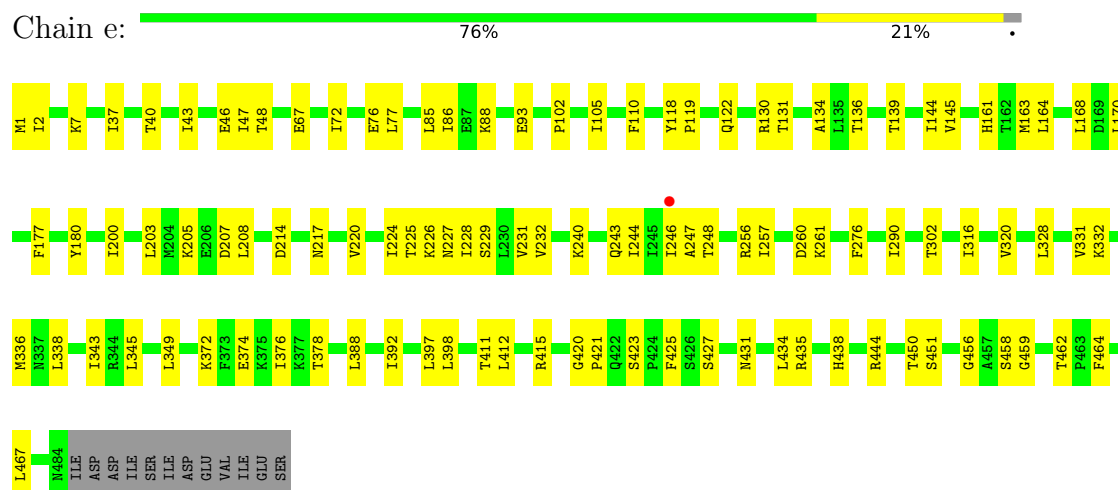
3 Residue-property plots

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: DNA-directed RNA polymerase beta subunit

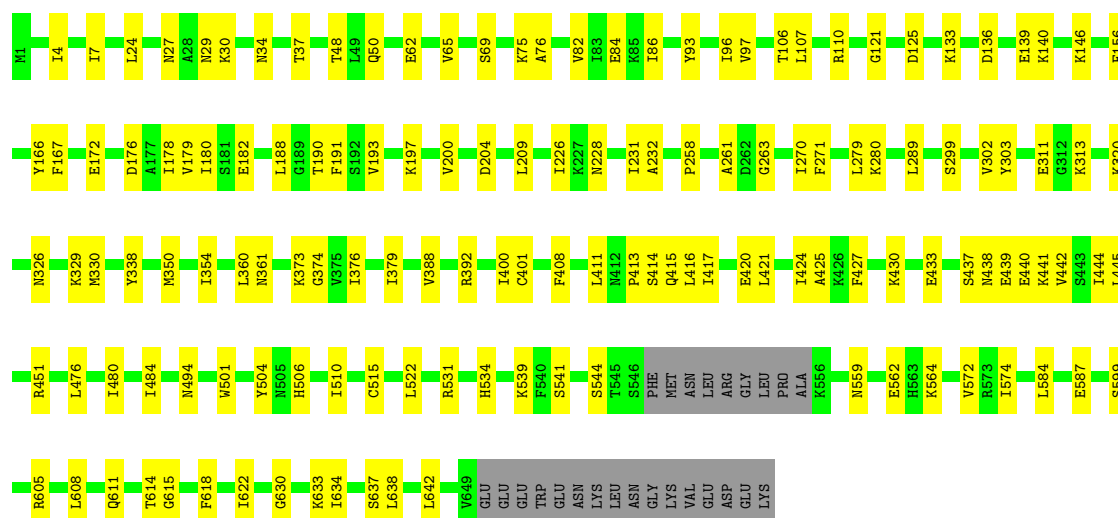


• Molecule 1: DNA-directed RNA polymerase beta subunit



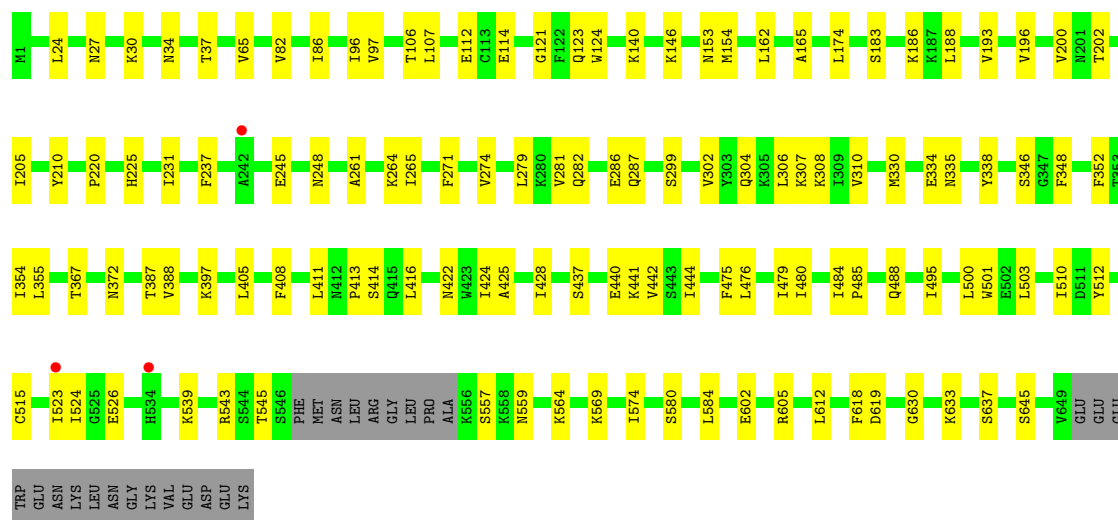
• Molecule 2: DNA-directed RNA polymerase





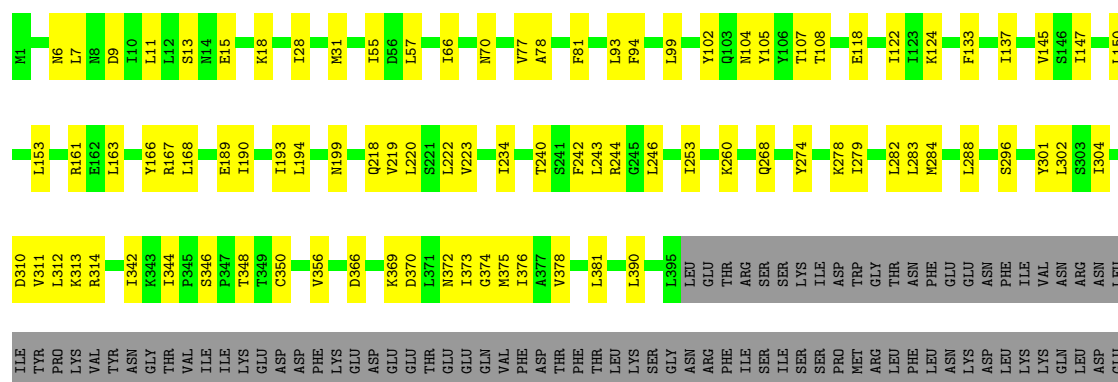
• Molecule 2: DNA-directed RNA polymerase

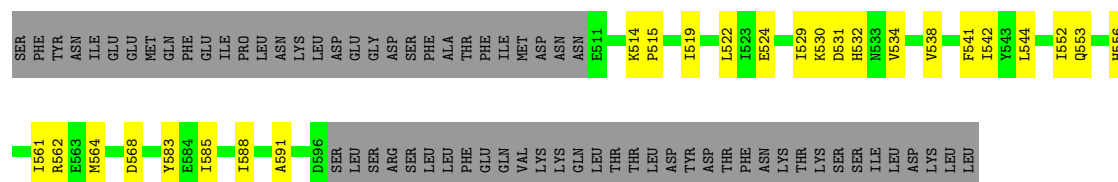
Chain E: 78% 18%



• Molecule 3: DNA-directed RNA polymerase

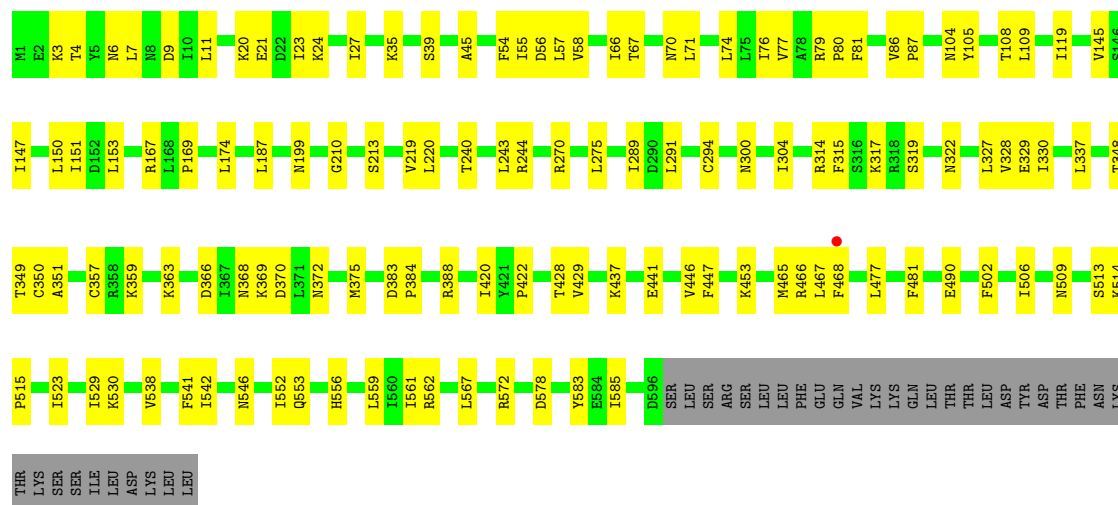
Chain D: 58% 18% 24%





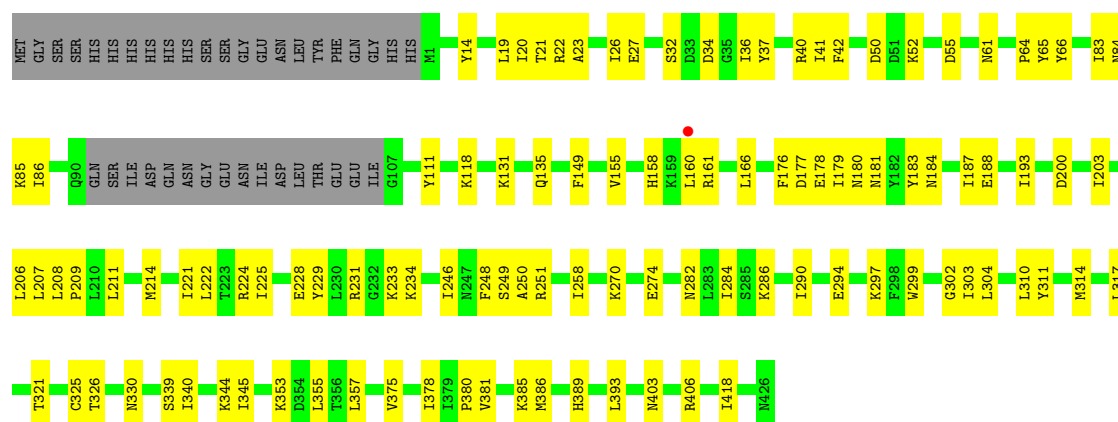
• Molecule 3: DNA-directed RNA polymerase

Chain F: 74% 20% 6%



• Molecule 4: DNA-directed RNA polymerase beta' subunit

Chain d: 67% 24% 8%



• Molecule 4: DNA-directed RNA polymerase beta' subunit

Chain f: 75% 17% 8%



I112	G113	L114	Y138	I142	H145	D146	S157	H158	R161	T164	T167	K172	A175	F176	I179	N180	I190	I193	V197	V198	D201	L206	L207	L208	P209	L210	L211	W214	I221	R224	I225	E228	G232	F236	N247	F248	S249
T255	M267	P268	Y269	K270	Q279	K288	E294	K297	E309	I310	Y311	N312	Y313	M314	E315	E316	T319	K320	T321	K322	G325	I337	I345	L355	G358	N361	D370	V375	K385	L399	R402	N403	R406	F407	D416	N426	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.86Å 166.27Å 307.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 3.30 49.42 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.42-3.30) 98.6 (49.42-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.219 , 0.258 0.218 , 0.258	Depositor DCC
R_{free} test set	4308 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	107.3	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 139.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33894	wwPDB-VP
Average B, all atoms (Å ²)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	c	0.14	0/4082	0.39	0/5502
1	e	0.14	0/4082	0.37	0/5502
2	C	0.15	0/5308	0.39	0/7156
2	E	0.13	0/5308	0.36	0/7156
3	D	0.10	0/3952	0.28	0/5328
3	F	0.11	0/4932	0.28	0/6650
4	d	0.14	1/3431 (0.0%)	0.35	0/4630
4	f	0.12	0/3431	0.33	0/4630
All	All	0.13	1/34526 (0.0%)	0.35	0/46554

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	357	LEU	C-N	-5.24	1.31	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	c	4003	0	4045	75	0
1	e	4003	0	4045	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5208	0	5085	106	0
2	E	5208	0	5085	88	0
3	D	3893	0	3932	79	0
3	F	4853	0	4850	84	0
4	d	3362	0	3371	86	0
4	f	3362	0	3371	59	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
All	All	33894	0	33784	587	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 9.

All (587) 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:E:425:ALA:HB1	2:E:484:ILE:HG21	1.49	0.92
3:F:477:LEU:HA	3:F:481:PHE:HB2	1.54	0.89
3:D:568:ASP:H	3:D:583:TYR:HA	1.42	0.85
4:d:179:ILE:HG12	4:d:224:ARG:HG2	1.57	0.84
4:f:179:ILE:HB	4:f:224:ARG:HG2	1.59	0.83
1:e:163:MET:HE2	1:e:247:ALA:HB2	1.65	0.78
1:e:450:THR:HG21	1:e:456:GLY:H	1.48	0.78
3:F:86:VAL:HG22	3:F:87:PRO:HD2	1.67	0.77
4:d:22:ARG:HH12	4:d:27:GLU:HB3	1.51	0.76
3:F:4:THR:HA	3:F:56:ASP:HB2	1.66	0.76
3:D:167:ARG:HH21	3:D:240:THR:HG22	1.50	0.76
4:d:200:ASP:HA	4:d:203:ILE:HG22	1.68	0.75
4:d:86:ILE:HA	4:d:111:TYR:HA	1.68	0.74
2:E:121:GLY:HA3	2:E:193:VAL:HG12	1.69	0.73
3:D:11:LEU:HD23	3:D:81:PHE:HB2	1.69	0.73
4:d:193:ILE:HG23	4:d:207:LEU:HD11	1.71	0.73
1:e:86:ILE:HD13	1:e:376:ILE:HD12	1.71	0.73
1:e:72:ILE:HD11	2:E:338:TYR:HB3	1.71	0.72
4:f:270:LYS:HD3	4:f:355:LEU:HD21	1.70	0.72
3:F:366:ASP:HA	3:F:369:LYS:HE3	1.72	0.72
3:F:6:ASN:HA	3:F:58:VAL:HB	1.71	0.71
2:E:245:GLU:HB3	2:E:248:ASN:HB2	1.72	0.71
1:e:67:GLU:HG3	2:E:335:ASN:HB3	1.72	0.71
2:E:545:THR:HG23	4:f:247:ASN:HD22	1.55	0.70
3:D:234:ILE:HD12	3:D:253:ILE:HG23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:374:GLU:O	1:c:378:THR:HG23	1.93	0.69
2:C:200:VAL:HG23	2:C:204:ASP:HB2	1.75	0.69
2:C:414:SER:HA	2:C:417:ILE:HD12	1.74	0.69
1:c:343:ILE:HD11	1:c:467:LEU:HD11	1.74	0.69
3:F:556:HIS:HA	3:F:559:LEU:HD12	1.75	0.69
2:E:645:SER:HB2	4:f:8:ILE:HD11	1.74	0.67
3:F:153:LEU:HD21	3:F:199:ASN:HB3	1.74	0.67
3:D:66:ILE:HG23	3:D:70:ASN:HB2	1.76	0.67
2:E:265:ILE:HG22	2:E:354:ILE:HG12	1.77	0.67
1:c:431:ASN:HB3	1:c:434:LEU:HB2	1.77	0.67
3:D:282:LEU:HD12	3:D:588:ILE:HD12	1.77	0.67
1:e:411:THR:HG23	1:e:412:LEU:HD23	1.76	0.66
2:C:360:LEU:HD21	2:C:376:ILE:HG13	1.75	0.66
3:D:529:ILE:HG23	3:D:585:ILE:HB	1.77	0.66
3:F:109:LEU:HG	3:F:119:ILE:HD11	1.77	0.66
2:C:121:GLY:HA3	2:C:193:VAL:HG12	1.78	0.65
4:d:166:LEU:HD22	4:f:206:LEU:HD12	1.76	0.65
3:D:153:LEU:HD13	3:D:199:ASN:HB3	1.79	0.65
1:c:88:LYS:HB3	1:c:373:PHE:HE1	1.62	0.65
1:e:343:ILE:HD11	1:e:467:LEU:HD11	1.78	0.65
3:F:348:THR:HA	3:F:562:ARG:HB2	1.78	0.65
1:c:462:THR:HG22	1:c:464:PHE:H	1.62	0.64
2:E:612:LEU:HG	4:f:279:GLN:HG2	1.80	0.64
2:C:27:ASN:HA	2:C:494:ASN:HD22	1.61	0.64
2:E:584:LEU:HD12	3:F:375:MET:HB3	1.78	0.64
4:f:164:THR:H	4:f:175:ALA:HB3	1.63	0.64
2:C:642:LEU:HD22	4:d:222:LEU:HD12	1.79	0.64
4:d:270:LYS:HD3	4:d:355:LEU:HD21	1.80	0.64
3:F:7:LEU:HD13	3:F:57:LEU:HD11	1.79	0.63
1:e:205:LYS:HB2	1:e:227:ASN:HA	1.81	0.63
4:d:50:ASP:HB3	4:d:52:LYS:HE2	1.81	0.62
2:C:361:ASN:HB3	4:d:353:LYS:HE2	1.80	0.62
2:E:220:PRO:HB2	2:E:265:ILE:HD13	1.82	0.62
2:C:425:ALA:HB1	2:C:484:ILE:HG21	1.82	0.62
4:f:311:TYR:HA	4:f:314:MET:HE2	1.81	0.62
1:c:72:ILE:HD11	2:C:338:TYR:HB3	1.80	0.62
1:e:131:THR:HG23	1:e:134:ALA:HB3	1.81	0.62
2:C:420:GLU:OE1	2:C:504:TYR:OH	2.15	0.61
2:C:313:LYS:HE3	2:C:313:LYS:HA	1.83	0.61
2:C:451:ARG:HH12	2:C:506:HIS:CD2	2.18	0.61
2:E:388:VAL:HA	2:E:515:CYS:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:425:PHE:HD1	1:e:431:ASN:HB2	1.65	0.61
3:D:366:ASP:HA	3:D:369:LYS:HE3	1.83	0.60
1:c:240:LYS:HB2	1:c:328:LEU:HD11	1.83	0.60
2:E:202:THR:HG23	2:E:346:SER:HB3	1.84	0.60
1:c:270:LYS:HD3	1:c:283:LYS:HB2	1.84	0.60
2:E:183:SER:HA	2:E:186:LYS:HE2	1.84	0.60
1:c:156:ILE:HD12	1:c:223:MET:HE2	1.84	0.60
3:F:567:LEU:HD23	3:F:583:TYR:HB3	1.84	0.59
4:d:66:TYR:HB2	4:d:118:LYS:HE2	1.84	0.59
3:F:74:LEU:HA	3:F:77:VAL:HG12	1.84	0.59
3:F:11:LEU:HD23	3:F:81:PHE:HB2	1.84	0.59
2:E:440:GLU:O	2:E:444:ILE:HG13	2.03	0.59
3:D:11:LEU:HD21	3:D:78:ALA:HB1	1.84	0.59
3:F:86:VAL:CG2	3:F:87:PRO:HD2	2.33	0.59
3:F:270:ARG:HE	3:F:441:GLU:HG2	1.67	0.59
1:c:372:LYS:O	1:c:376:ILE:HG12	2.03	0.59
2:C:388:VAL:HA	2:C:515:CYS:HA	1.83	0.59
2:C:416:LEU:O	2:C:420:GLU:HG2	2.02	0.58
4:f:179:ILE:HG13	4:f:221:ILE:HG12	1.83	0.58
3:F:372:ASN:HB3	3:F:375:MET:HB2	1.85	0.58
2:E:422:ASN:ND2	2:E:526:GLU:O	2.35	0.58
3:F:167:ARG:HH21	3:F:240:THR:HG22	1.69	0.58
2:E:559:ASN:HB3	2:E:564:LYS:HB2	1.85	0.58
1:c:270:LYS:HE2	1:c:284:GLN:HG3	1.86	0.58
1:c:408:SER:HA	1:c:411:THR:HG22	1.86	0.58
2:C:539:LYS:HB3	4:d:375:VAL:HG11	1.85	0.57
2:E:476:LEU:O	2:E:480:ILE:HG12	2.04	0.57
1:e:392:ILE:HG23	1:e:398:LEU:HD13	1.86	0.57
3:F:317:LYS:HB3	3:F:363:LYS:HB2	1.86	0.57
4:d:381:VAL:HG23	4:d:386:MET:HE3	1.86	0.57
4:f:176:PHE:HB2	4:f:180:ASN:HB2	1.85	0.57
4:f:142:ILE:HA	4:f:145:HIS:CE1	2.40	0.57
2:E:86:ILE:HD12	2:E:302:VAL:HG12	1.86	0.57
1:c:305:ILE:HG23	1:c:474:HIS:HE1	1.70	0.57
1:c:468:PRO:HD2	1:c:474:HIS:O	2.05	0.57
2:C:188:LEU:HB3	2:C:360:LEU:HD12	1.87	0.56
2:E:162:LEU:HD11	2:E:188:LEU:HD21	1.86	0.56
1:e:240:LYS:O	1:e:244:ILE:HG13	2.06	0.56
4:f:63:GLU:HG2	4:f:64:PRO:HA	1.87	0.56
2:C:167:PHE:HB2	2:C:522:LEU:HD21	1.86	0.56
2:E:210:TYR:CE2	2:E:220:PRO:HG3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:168:LEU:HG	3:D:222:LEU:HD11	1.88	0.56
3:D:519:ILE:HG12	3:D:544:LEU:HB3	1.88	0.56
3:D:279:ILE:HG22	3:D:378:VAL:HG12	1.87	0.56
3:F:289:ILE:HD13	3:F:291:LEU:HB3	1.87	0.56
3:D:147:ILE:HG23	3:D:243:LEU:HD21	1.88	0.56
4:d:42:PHE:HB3	4:d:158:HIS:HD2	1.71	0.56
1:e:118:TYR:CG	1:e:412:LEU:HD12	2.41	0.56
4:d:22:ARG:NH1	4:d:27:GLU:HB3	2.19	0.56
3:F:77:VAL:HG22	3:F:105:TYR:CE2	2.41	0.56
3:F:351:ALA:HA	3:F:572:ARG:HB3	1.88	0.56
3:D:77:VAL:HG22	3:D:105:TYR:HE2	1.72	0.55
1:e:224:ILE:HB	1:e:228:ILE:HB	1.88	0.55
2:C:180:ILE:HG13	2:C:400:ILE:HG22	1.88	0.55
2:C:280:LYS:HA	2:C:289:LEU:HD21	1.89	0.55
3:F:446:VAL:HG12	3:F:468:PHE:HE1	1.71	0.55
3:D:167:ARG:NH2	3:D:240:THR:HG22	2.21	0.55
4:d:203:ILE:HG12	4:d:206:LEU:HD11	1.89	0.55
1:e:200:ILE:HA	1:e:231:VAL:O	2.07	0.55
2:C:584:LEU:HD12	3:D:375:MET:HB3	1.89	0.54
1:e:144:ILE:HD11	1:e:320:VAL:HG22	1.89	0.54
2:C:226:ILE:HD13	2:C:231:ILE:HG12	1.88	0.54
1:e:214:ASP:HA	1:e:217:ASN:ND2	2.22	0.54
2:C:93:TYR:CD2	2:C:110:ARG:HD2	2.42	0.54
4:d:325:CYS:HB3	4:d:345:ILE:HD12	1.88	0.54
2:E:441:LYS:HD2	2:E:476:LEU:HD23	1.90	0.54
4:d:131:LYS:O	4:d:135:GLN:HB2	2.07	0.54
3:F:314:ARG:NH2	3:F:546:ASN:OD1	2.41	0.54
3:F:553:GLN:HG3	4:f:403:ASN:O	2.08	0.54
4:f:190:ILE:HG23	4:f:214:MET:SD	2.48	0.54
2:C:360:LEU:HA	2:C:531:ARG:HH21	1.73	0.53
1:e:2:ILE:HG23	2:E:485:PRO:HG3	1.90	0.53
1:e:220:VAL:HG23	1:e:232:VAL:HB	1.90	0.53
2:E:602:GLU:O	2:E:605:ARG:HG2	2.08	0.53
2:C:559:ASN:HB3	2:C:564:LYS:HB2	1.90	0.53
3:D:561:ILE:HA	3:D:564:MET:HE2	1.90	0.53
2:E:281:VAL:HG13	2:E:282:GLN:HG3	1.91	0.53
3:F:529:ILE:HG23	3:F:585:ILE:HB	1.90	0.53
3:F:294:CYS:HB2	3:F:351:ALA:HB3	1.89	0.53
4:f:288:LYS:NZ	4:f:309:GLU:OE2	2.29	0.53
1:e:164:LEU:O	1:e:244:ILE:HA	2.08	0.53
1:c:221:ILE:HG12	1:c:231:VAL:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:374:GLU:O	1:e:378:THR:HG23	2.08	0.53
4:d:250:ALA:HB3	4:d:378:ILE:HB	1.90	0.53
3:F:300:ASN:HD21	3:F:349:THR:HB	1.73	0.53
2:E:114:GLU:HB2	2:E:124:TRP:HE1	1.74	0.53
1:c:257:ILE:HD12	1:c:262:ILE:HD11	1.90	0.53
2:C:445:LEU:HD11	2:C:484:ILE:CD1	2.38	0.53
2:E:96:ILE:HD13	2:E:306:LEU:HD21	1.91	0.53
2:E:484:ILE:HD12	2:E:485:PRO:HD2	1.91	0.53
4:f:114:LEU:HD23	4:f:211:LEU:HD23	1.90	0.53
3:F:147:ILE:HD13	3:F:243:LEU:HD11	1.90	0.53
2:C:599:SER:O	2:C:605:ARG:NH2	2.43	0.52
3:D:28:ILE:HA	3:D:31:MET:HE2	1.92	0.52
4:f:138:TYR:O	4:f:142:ILE:HG12	2.10	0.52
1:c:357:PHE:O	1:c:361:THR:HG23	2.10	0.52
2:C:299:SER:O	2:C:302:VAL:HG22	2.09	0.52
1:e:462:THR:HG22	1:e:464:PHE:H	1.73	0.52
2:E:299:SER:O	2:E:302:VAL:HG22	2.10	0.52
2:E:501:TRP:CE2	3:F:151:ILE:HG23	2.44	0.52
4:f:294:GLU:HA	4:f:297:LYS:HE2	1.90	0.52
2:C:642:LEU:HD21	4:d:225:ILE:HB	1.91	0.52
1:c:196:LEU:HD22	1:c:236:PHE:HE2	1.75	0.52
2:E:27:ASN:HB3	2:E:30:LYS:HD2	1.92	0.52
3:F:428:THR:HB	3:F:453:LYS:HB3	1.91	0.52
3:F:54:PHE:HA	3:F:67:THR:HA	1.92	0.52
3:D:288:LEU:HD13	3:D:373:ILE:HG13	1.90	0.52
1:c:286:LYS:O	1:c:290:ILE:HG12	2.10	0.52
2:E:231:ILE:HD11	2:E:261:ALA:HB3	1.91	0.51
2:E:416:LEU:HD21	3:F:145:VAL:HG12	1.92	0.51
2:E:424:ILE:O	2:E:428:ILE:HG12	2.09	0.51
1:e:46:GLU:HA	1:e:88:LYS:HD3	1.93	0.51
1:c:462:THR:HG22	1:c:464:PHE:N	2.26	0.51
3:D:194:LEU:HA	3:D:199:ASN:HD21	1.75	0.51
1:e:316:ILE:O	1:e:320:VAL:HG23	2.10	0.51
3:F:66:ILE:HG23	3:F:70:ASN:HB2	1.91	0.51
3:D:268:GLN:HG2	3:D:390:LEU:HG	1.92	0.51
3:F:446:VAL:HG12	3:F:468:PHE:CE1	2.44	0.51
2:C:279:LEU:HB3	2:C:289:LEU:HD11	1.91	0.51
1:e:427:SER:HA	1:e:435:ARG:HH22	1.74	0.51
2:C:303:TYR:HE1	2:C:329:LYS:HE3	1.76	0.51
4:f:325:CYS:HB3	4:f:345:ILE:HD12	1.93	0.51
3:D:304:ILE:HD11	3:D:542:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:82:VAL:HA	2:E:97:VAL:HG12	1.92	0.51
2:C:179:VAL:HG23	2:C:401:CYS:HB2	1.93	0.51
1:e:338:LEU:HD12	1:e:444:ARG:HD2	1.93	0.51
3:F:270:ARG:NE	3:F:441:GLU:HG2	2.25	0.51
2:C:84:GLU:HB2	2:C:96:ILE:HD11	1.93	0.50
2:E:405:LEU:HD12	4:f:416:ASP:OD2	2.12	0.50
1:c:88:LYS:HG2	1:c:89:ASP:H	1.77	0.50
2:C:440:GLU:O	2:C:444:ILE:HG13	2.11	0.50
2:C:574:ILE:HG13	4:d:246:ILE:HD13	1.92	0.50
3:D:350:CYS:SG	3:D:356:VAL:HA	2.51	0.50
3:F:275:LEU:HD21	3:F:523:ILE:HD11	1.93	0.50
2:C:445:LEU:HD11	2:C:484:ILE:HD11	1.92	0.50
4:d:161:ARG:HD2	4:d:180:ASN:ND2	2.26	0.50
1:e:336:MET:HE2	1:e:438:HIS:HB2	1.93	0.50
1:e:420:GLY:H	1:e:423:SER:HB3	1.76	0.50
4:d:299:TRP:CZ2	4:d:303:ILE:HD11	2.47	0.50
2:C:541:SER:HB3	4:d:251:ARG:HB2	1.94	0.50
1:c:137:LEU:HB3	1:c:144:ILE:HG23	1.93	0.50
1:c:336:MET:HE2	1:c:438:HIS:HB2	1.94	0.50
2:C:270:ILE:HG13	2:C:350:MET:HG2	1.92	0.50
3:D:93:LEU:HD23	3:D:94:PHE:N	2.27	0.50
1:c:134:ALA:HA	1:c:146:LEU:O	2.12	0.50
4:d:284:ILE:HG22	4:d:290:ILE:HD11	1.94	0.50
3:F:466:ARG:HB2	3:F:506:ILE:HD12	1.94	0.50
1:e:431:ASN:HB3	1:e:434:LEU:HD23	1.94	0.49
2:E:630:GLY:HA2	2:E:633:LYS:HE2	1.95	0.49
4:d:161:ARG:HH11	4:d:180:ASN:HD22	1.60	0.49
2:C:476:LEU:O	2:C:480:ILE:HG12	2.13	0.49
2:C:572:VAL:HB	4:d:249:SER:HB2	1.93	0.49
2:C:615:GLY:O	4:d:282:ASN:ND2	2.46	0.49
4:d:176:PHE:HB2	4:d:180:ASN:OD1	2.12	0.49
4:f:370:ASP:OD1	4:f:370:ASP:N	2.45	0.49
3:F:6:ASN:HB3	3:F:9:ASP:HB2	1.94	0.49
2:E:112:GLU:O	2:E:124:TRP:N	2.45	0.49
2:E:174:LEU:HD13	4:f:361:ASN:ND2	2.28	0.49
1:c:408:SER:N	2:C:69:SER:OG	2.39	0.49
2:C:125:ASP:HB3	2:C:146:LYS:HG2	1.94	0.49
3:D:524:GLU:HA	3:D:588:ILE:HG22	1.94	0.49
4:d:248:PHE:O	4:d:380:PRO:HD2	2.12	0.49
1:e:48:THR:HB	1:e:85:LEU:O	2.13	0.49
1:e:208:LEU:HD22	1:e:229:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:146:ASP:N	4:f:146:ASP:OD1	2.44	0.49
4:d:40:ARG:HG3	4:d:41:ILE:HG23	1.94	0.49
2:E:637:SER:HB3	4:f:57:ILE:HD11	1.94	0.49
3:D:314:ARG:HD2	3:D:552:ILE:O	2.13	0.48
2:E:387:THR:HG22	2:E:397:LYS:HG2	1.94	0.48
3:F:541:PHE:HD2	3:F:561:ILE:HD11	1.77	0.48
2:C:34:ASN:O	2:C:37:THR:HG22	2.13	0.48
2:E:416:LEU:HD23	3:F:147:ILE:HG13	1.95	0.48
3:F:169:PRO:HD2	3:F:174:LEU:HD11	1.95	0.48
3:D:381:LEU:HA	3:D:552:ILE:HD11	1.95	0.48
3:F:153:LEU:HD11	3:F:199:ASN:HB3	1.94	0.48
3:F:384:PRO:O	3:F:388:ARG:HB2	2.13	0.48
3:D:99:LEU:HD22	4:d:418:ILE:HG23	1.94	0.48
1:e:214:ASP:HA	1:e:217:ASN:HD21	1.77	0.48
2:E:512:TYR:HD1	2:E:523:ILE:HG23	1.77	0.48
2:E:539:LYS:HB3	4:f:375:VAL:HG11	1.95	0.48
3:F:20:LYS:HD2	3:F:76:ILE:HG12	1.94	0.48
3:F:150:LEU:HD11	3:F:220:LEU:HD21	1.96	0.48
2:C:311:GLU:OE2	2:C:329:LYS:NZ	2.42	0.48
1:c:360:GLY:HA3	1:c:379:ILE:HG23	1.96	0.48
3:F:304:ILE:HG21	3:F:315:PHE:CZ	2.48	0.48
1:c:81:LYS:HB2	1:c:98:PHE:HE1	1.77	0.48
2:E:193:VAL:HA	2:E:354:ILE:O	2.13	0.48
2:C:27:ASN:HB2	2:C:414:SER:OG	2.14	0.48
3:D:77:VAL:HG22	3:D:105:TYR:CE2	2.48	0.48
4:f:26:ILE:HD13	4:f:31:PHE:HA	1.95	0.48
2:C:427:PHE:CG	2:C:510:ILE:HG12	2.48	0.48
2:E:367:THR:HB	2:E:372:ASN:O	2.14	0.48
1:c:36:PRO:O	1:c:40:THR:HG23	2.14	0.48
2:C:226:ILE:HG13	2:C:263:GLY:O	2.14	0.48
2:C:392:ARG:HH21	2:C:430:LYS:HB3	1.77	0.48
4:d:183:TYR:O	4:d:187:ILE:HG13	2.14	0.48
2:E:205:ILE:HG12	2:E:237:PHE:HE2	1.79	0.48
1:c:194:PHE:HB3	1:c:196:LEU:HG	1.95	0.47
1:c:316:ILE:O	1:c:320:VAL:HG23	2.14	0.47
1:e:76:GLU:HB3	1:e:105:ILE:HD11	1.96	0.47
2:E:24:LEU:HD11	2:E:65:VAL:HG21	1.96	0.47
3:F:429:VAL:O	3:F:490:GLU:HA	2.14	0.47
2:C:424:ILE:HG13	2:C:510:ILE:HD13	1.95	0.47
3:D:55:ILE:HG13	3:D:66:ILE:O	2.14	0.47
4:d:66:TYR:HB3	4:d:149:PHE:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:447:PHE:CZ	3:F:467:LEU:HB2	2.49	0.47
2:C:93:TYR:CE2	2:C:110:ARG:HD2	2.49	0.47
2:E:114:GLU:HB2	2:E:124:TRP:NE1	2.29	0.47
3:F:319:SER:HA	3:F:329:GLU:HA	1.97	0.47
1:c:177:PHE:CD1	1:c:248:THR:HG21	2.49	0.47
2:C:438:ASN:O	2:C:442:VAL:HG13	2.13	0.47
2:E:618:PHE:CD1	4:f:320:LYS:HB2	2.48	0.47
3:F:330:ILE:HD11	3:F:337:LEU:HD13	1.94	0.47
2:E:619:ASP:HB2	4:f:322:LYS:HD3	1.95	0.47
1:c:407:ILE:HG12	2:C:156:PHE:HZ	1.79	0.47
4:d:161:ARG:HB2	4:d:180:ASN:HD21	1.78	0.47
1:c:118:TYR:CB	1:c:412:LEU:HD12	2.45	0.47
1:c:287:GLY:O	1:c:291:ILE:HG13	2.15	0.47
1:c:411:THR:HG23	1:c:412:LEU:HD23	1.97	0.47
3:D:534:VAL:O	3:D:538:VAL:HG12	2.14	0.47
1:e:136:THR:OG1	1:e:145:VAL:HG22	2.14	0.47
2:E:405:LEU:HD22	3:F:210:GLY:HA3	1.97	0.47
3:F:55:ILE:HD11	3:F:71:LEU:HB2	1.96	0.47
4:f:221:ILE:O	4:f:225:ILE:HG12	2.15	0.47
4:f:312:ASN:O	4:f:316:GLU:HG2	2.15	0.47
4:d:311:TYR:HA	4:d:314:MET:HE2	1.97	0.47
1:e:47:ILE:HD11	1:e:376:ILE:HB	1.97	0.47
2:E:488:GLN:HE22	2:E:495:ILE:HG23	1.79	0.47
2:E:500:LEU:HA	2:E:503:LEU:HD12	1.96	0.47
1:c:72:ILE:HD12	2:C:271:PHE:CD1	2.50	0.47
1:c:106:ASP:HB2	1:c:109:TYR:CE2	2.50	0.47
2:C:86:ILE:HD13	2:C:302:VAL:HG12	1.97	0.47
2:C:193:VAL:HA	2:C:354:ILE:O	2.14	0.47
1:e:7:LYS:HD3	2:E:153:ASN:HB3	1.96	0.47
1:e:372:LYS:O	1:e:376:ILE:HG12	2.15	0.47
2:E:34:ASN:O	2:E:37:THR:HG22	2.15	0.47
1:e:130:ARG:HG2	1:e:131:THR:N	2.29	0.46
1:c:228:ILE:HG12	1:c:259:ILE:HG13	1.96	0.46
1:c:305:ILE:HG23	1:c:474:HIS:CE1	2.49	0.46
4:d:229:TYR:HD1	4:d:233:LYS:HB3	1.79	0.46
2:E:334:GLU:HG2	2:E:335:ASN:H	1.81	0.46
3:D:99:LEU:HA	3:D:102:TYR:CD1	2.50	0.46
3:D:167:ARG:CZ	3:D:244:ARG:HH21	2.28	0.46
4:d:193:ILE:HD12	4:d:214:MET:HE1	1.96	0.46
3:F:21:GLU:HA	3:F:24:LYS:HE2	1.96	0.46
1:c:46:GLU:HG3	1:c:88:LYS:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:294:GLU:HA	4:d:297:LYS:HE2	1.97	0.46
1:e:349:LEU:HD21	1:e:398:LEU:HD11	1.98	0.46
3:F:79:ARG:N	3:F:80:PRO:HD2	2.30	0.46
1:c:225:THR:HG22	1:c:226:LYS:N	2.31	0.46
4:f:142:ILE:HG23	4:f:145:HIS:HE1	1.80	0.46
3:F:370:ASP:OD1	3:F:370:ASP:N	2.49	0.46
2:C:608:LEU:HD13	2:C:622:ILE:HD13	1.97	0.46
3:D:104:ASN:O	3:D:108:THR:HG23	2.14	0.46
1:e:397:LEU:HD22	1:e:421:PRO:HG3	1.98	0.46
3:F:187:LEU:HD21	3:F:213:SER:HB3	1.98	0.46
4:f:164:THR:N	4:f:175:ALA:HB3	2.29	0.46
3:D:118:GLU:O	3:D:122:ILE:HG12	2.15	0.46
3:D:541:PHE:HD2	3:D:561:ILE:HD11	1.80	0.46
3:F:314:ARG:HD2	3:F:552:ILE:O	2.16	0.46
3:D:6:ASN:HB3	3:D:9:ASP:HB2	1.97	0.45
3:D:260:LYS:HB3	3:D:260:LYS:HE2	1.78	0.45
3:D:530:LYS:HE3	1:e:256:ARG:HH22	1.82	0.45
2:E:557:SER:HB2	2:E:569:LYS:H	1.81	0.45
1:c:118:TYR:HB2	1:c:412:LEU:HD12	1.99	0.45
2:C:29:ASN:OD1	2:C:29:ASN:N	2.47	0.45
2:C:231:ILE:HD11	2:C:261:ALA:HB3	1.98	0.45
4:d:161:ARG:HH11	4:d:180:ASN:ND2	2.14	0.45
2:E:424:ILE:HG13	2:E:510:ILE:CD1	2.47	0.45
1:c:124:LEU:HD23	1:c:124:LEU:HA	1.86	0.45
1:c:285:GLU:O	1:c:288:GLU:HG2	2.17	0.45
1:c:327:TYR:O	1:c:331:VAL:HG23	2.16	0.45
2:C:176:ASP:HB3	2:C:373:LYS:O	2.16	0.45
3:D:370:ASP:OD1	3:D:370:ASP:N	2.50	0.45
3:D:515:PRO:O	3:D:519:ILE:HG13	2.16	0.45
4:d:228:GLU:HG2	4:d:231:ARG:HH22	1.82	0.45
1:e:170:LEU:HD23	1:e:170:LEU:HA	1.82	0.45
1:c:411:THR:O	1:c:412:LEU:HD22	2.16	0.45
2:C:29:ASN:O	3:D:246:LEU:HB2	2.17	0.45
4:d:330:ASN:HA	4:d:339:SER:O	2.16	0.45
4:d:385:LYS:HB3	4:d:385:LYS:HE3	1.82	0.45
3:F:368:ASN:HD22	4:f:402:ARG:HG3	1.81	0.45
3:F:383:ASP:HB3	3:F:384:PRO:HD3	1.99	0.45
2:C:182:GLU:HA	2:C:379:ILE:HD11	1.98	0.45
2:C:411:LEU:C	2:C:413:PRO:HD3	2.42	0.45
2:C:425:ALA:HB1	2:C:484:ILE:CG2	2.44	0.45
2:E:304:GLN:HA	2:E:307:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:584:LEU:HD21	4:f:337:ILE:HG22	1.99	0.45
4:f:86:ILE:HG23	4:f:112:ILE:HG13	1.99	0.45
4:f:197:VAL:HG23	4:f:198:VAL:H	1.82	0.45
2:C:121:GLY:HA3	2:C:193:VAL:CG1	2.44	0.45
2:C:630:GLY:HA2	2:C:633:LYS:HE3	1.99	0.45
4:d:282:ASN:O	4:d:286:LYS:HG2	2.17	0.45
3:F:422:PRO:HG3	3:F:502:PHE:HB2	1.99	0.45
3:D:15:GLU:HG2	3:D:18:LYS:HB3	1.97	0.45
4:d:340:ILE:HG23	4:d:393:LEU:HD13	1.98	0.45
1:e:332:LYS:HE3	1:e:332:LYS:HB2	1.84	0.45
3:F:327:LEU:HD23	3:F:359:LYS:NZ	2.31	0.45
2:C:408:PHE:HD1	3:D:219:VAL:HG11	1.81	0.45
4:d:85:LYS:HB3	4:d:111:TYR:CE1	2.52	0.45
4:d:211:LEU:HA	4:d:214:MET:SD	2.57	0.45
2:E:501:TRP:CE3	3:F:151:ILE:HG12	2.52	0.45
3:F:578:ASP:OD1	3:F:578:ASP:N	2.50	0.45
2:C:611:GLN:HA	2:C:614:THR:HG22	1.99	0.44
1:e:328:LEU:O	1:e:332:LYS:HE2	2.17	0.44
2:E:27:ASN:HB2	2:E:414:SER:OG	2.17	0.44
2:E:200:VAL:HG11	2:E:348:PHE:CZ	2.52	0.44
3:F:3:LYS:HA	3:F:3:LYS:HD2	1.79	0.44
4:f:63:GLU:CG	4:f:64:PRO:HA	2.47	0.44
2:C:24:LEU:HD21	2:C:65:VAL:HG21	1.99	0.44
1:c:342:ARG:HB3	1:c:474:HIS:CD2	2.53	0.44
1:c:431:ASN:O	1:c:435:ARG:HG3	2.18	0.44
2:C:29:ASN:OD1	2:C:494:ASN:ND2	2.51	0.44
2:C:433:GLU:HB2	2:C:480:ILE:HG21	2.00	0.44
2:C:544:SER:HB3	4:d:274:GLU:O	2.18	0.44
2:C:562:GLU:HB3	2:C:564:LYS:HZ3	1.82	0.44
3:D:218:GLN:HG2	3:D:223:VAL:HA	1.98	0.44
3:D:342:ILE:HD12	3:D:344:ILE:HD11	2.00	0.44
1:c:156:ILE:HA	1:c:223:MET:HE3	1.99	0.44
2:C:30:LYS:O	2:C:413:PRO:HD2	2.18	0.44
4:d:23:ALA:HB1	4:d:188:GLU:HG3	1.99	0.44
2:E:306:LEU:O	2:E:310:VAL:HG23	2.18	0.44
2:C:326:ASN:O	2:C:330:MET:HG3	2.17	0.44
3:D:296:SER:HB2	3:D:301:TYR:HE1	1.82	0.44
4:d:208:LEU:HD13	4:d:211:LEU:HD12	1.99	0.44
3:F:300:ASN:ND2	3:F:349:THR:HB	2.32	0.44
4:f:309:GLU:HG2	4:f:313:TYR:CE2	2.52	0.44
1:c:175:VAL:HB	1:c:180:TYR:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:348:THR:HA	3:D:562:ARG:HB2	1.99	0.44
1:e:119:PRO:HB2	1:e:345:LEU:HD11	2.00	0.44
2:E:286:GLU:HG3	2:E:287:GLN:N	2.33	0.44
1:c:246:ILE:O	1:c:250:LEU:HG	2.18	0.44
1:c:411:THR:C	1:c:412:LEU:HD22	2.43	0.44
1:e:225:THR:HG22	1:e:226:LYS:H	1.83	0.44
4:d:14:TYR:HE1	4:d:19:LEU:HD13	1.82	0.44
4:d:64:PRO:HD2	4:d:65:TYR:CE2	2.53	0.44
1:e:168:LEU:HD21	1:e:170:LEU:HD12	2.00	0.44
4:f:179:ILE:HD11	4:f:221:ILE:HG23	2.00	0.44
4:f:385:LYS:HE3	4:f:385:LYS:HB3	1.87	0.44
2:C:587:GLU:HG2	4:d:389:HIS:CG	2.53	0.44
4:d:181:ASN:HA	4:d:184:ASN:ND2	2.32	0.44
1:e:110:PHE:HD2	1:e:398:LEU:HD21	1.83	0.44
1:e:425:PHE:CD1	1:e:431:ASN:HB2	2.50	0.44
2:C:451:ARG:HH22	2:C:506:HIS:CE1	2.36	0.43
2:C:634:ILE:HG12	4:d:160:LEU:HD21	1.99	0.43
2:C:637:SER:OG	4:d:55:ASP:HA	2.18	0.43
4:d:19:LEU:HG	4:d:21:THR:HG23	2.00	0.43
4:d:155:VAL:HG23	4:d:183:TYR:CE2	2.54	0.43
1:c:37:ILE:HG12	1:c:354:LEU:HD12	2.00	0.43
3:D:189:GLU:O	3:D:193:ILE:HG12	2.18	0.43
2:E:308:LYS:HA	2:E:308:LYS:HD2	1.70	0.43
2:E:442:VAL:HG12	2:E:476:LEU:HD11	1.99	0.43
3:F:167:ARG:HG2	3:F:244:ARG:HH12	1.82	0.43
1:c:144:ILE:HD11	1:c:320:VAL:HG22	2.01	0.43
2:C:4:ILE:HG13	2:C:7:ILE:HD12	2.00	0.43
2:C:494:ASN:OD1	2:C:494:ASN:N	2.51	0.43
3:D:9:ASP:O	3:D:13:SER:HB3	2.18	0.43
3:D:163:LEU:HD13	3:D:190:ILE:HG13	2.01	0.43
4:d:155:VAL:HG23	4:d:183:TYR:CZ	2.53	0.43
1:e:260:ASP:OD2	1:e:261:LYS:N	2.51	0.43
3:D:372:ASN:O	3:D:376:ILE:HG12	2.18	0.43
3:F:514:LYS:HB2	3:F:515:PRO:HD3	2.00	0.43
4:f:319:THR:HB	4:f:320:LYS:HZ2	1.83	0.43
3:D:167:ARG:NE	3:D:244:ARG:HH21	2.16	0.43
4:d:317:LEU:O	4:d:321:THR:OG1	2.32	0.43
1:e:415:ARG:HD3	1:e:459:GLY:O	2.18	0.43
2:C:228:ASN:HB3	4:d:304:LEU:HD13	1.99	0.43
3:D:166:TYR:O	3:D:244:ARG:NH2	2.52	0.43
4:d:20:ILE:HD13	4:d:36:ILE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:225:HIS:CD2	2:E:264:LYS:HB2	2.54	0.43
3:F:368:ASN:ND2	4:f:402:ARG:HG3	2.34	0.43
4:f:24:ASN:ND2	4:f:26:ILE:O	2.51	0.43
1:c:184:LYS:HD2	1:c:317:TYR:CZ	2.54	0.43
1:c:298:LEU:HD23	1:c:303:LYS:HE2	2.00	0.43
2:C:539:LYS:HE2	4:d:375:VAL:HG21	2.00	0.43
3:D:553:GLN:HG3	4:d:403:ASN:O	2.19	0.43
1:e:177:PHE:CD1	1:e:248:THR:HG21	2.54	0.43
2:E:274:VAL:HG21	2:E:279:LEU:HD21	1.99	0.43
1:c:133:LYS:O	1:c:147:ARG:HD3	2.19	0.43
2:C:421:LEU:O	2:C:424:ILE:HG22	2.18	0.43
2:C:638:LEU:HD22	4:d:225:ILE:HD12	2.01	0.43
1:e:388:LEU:HD23	1:e:388:LEU:HA	1.84	0.43
2:E:146:LYS:HD3	2:E:154:MET:HE1	2.01	0.43
2:C:106:THR:HG22	2:C:107:LEU:H	1.84	0.43
4:d:158:HIS:HA	4:d:161:ARG:HG3	2.00	0.43
1:e:208:LEU:HD13	1:e:229:SER:OG	2.19	0.43
2:E:543:ARG:HB3	4:f:249:SER:H	1.84	0.43
4:f:172:LYS:HD3	4:f:172:LYS:HA	1.77	0.43
1:c:136:THR:HG23	1:c:145:VAL:HG22	2.00	0.42
1:e:72:ILE:HD12	2:E:271:PHE:CD1	2.54	0.42
1:c:286:LYS:HA	1:c:286:LYS:HD2	1.87	0.42
1:e:168:LEU:HD23	1:e:180:TYR:CE1	2.54	0.42
1:e:331:VAL:HG13	1:e:332:LYS:HG3	2.00	0.42
2:E:475:PHE:CZ	2:E:479:ILE:HD11	2.55	0.42
3:D:7:LEU:HB2	3:D:57:LEU:HD11	2.00	0.42
3:D:274:TYR:O	3:D:278:LYS:HG2	2.20	0.42
4:d:19:LEU:HD11	4:d:61:ASN:HB2	2.00	0.42
4:d:302:GLY:HA3	4:d:310:LEU:HD22	2.01	0.42
1:e:276:PHE:CE2	1:e:290:ILE:HG13	2.54	0.42
2:E:574:ILE:HD13	2:E:574:ILE:HA	1.91	0.42
4:f:190:ILE:O	4:f:193:ILE:HG12	2.18	0.42
4:f:316:GLU:O	4:f:320:LYS:HG2	2.19	0.42
1:c:363:ARG:HD3	4:f:145:HIS:ND1	2.35	0.42
1:c:420:GLY:H	1:c:423:SER:HB3	1.83	0.42
3:D:538:VAL:O	3:D:542:ILE:HG23	2.18	0.42
4:d:206:LEU:O	4:d:209:PRO:HD2	2.20	0.42
4:d:221:ILE:O	4:d:225:ILE:HG12	2.19	0.42
3:F:81:PHE:HB3	3:F:86:VAL:O	2.19	0.42
3:F:465:MET:HB3	3:F:506:ILE:O	2.19	0.42
4:f:232:GLY:O	4:f:236:PHE:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:150:LEU:HD21	3:D:220:LEU:HG	2.00	0.42
2:E:484:ILE:HD12	2:E:485:PRO:CD	2.49	0.42
3:F:437:LYS:O	3:F:446:VAL:HG22	2.19	0.42
1:c:88:LYS:HG2	1:c:89:ASP:N	2.34	0.42
1:c:173:SER:HB2	1:c:276:PHE:CE1	2.55	0.42
2:C:178:ILE:HD11	2:C:374:GLY:HA3	2.02	0.42
2:C:258:PRO:O	2:C:564:LYS:HA	2.19	0.42
4:d:27:GLU:HG2	4:d:32:SER:HA	2.02	0.42
2:E:165:ALA:HB2	2:E:524:ILE:HG12	2.01	0.42
3:F:23:ILE:O	3:F:27:ILE:HG13	2.19	0.42
1:c:388:LEU:HD23	1:c:388:LEU:HA	1.94	0.42
2:C:50:GLN:HG2	2:C:191:PHE:CZ	2.54	0.42
2:E:411:LEU:C	2:E:413:PRO:HD3	2.44	0.42
2:C:209:LEU:HD12	2:C:232:ALA:HA	2.02	0.42
3:F:39:SER:HB3	3:F:45:ALA:HB2	2.01	0.42
3:F:538:VAL:O	3:F:542:ILE:HG23	2.20	0.42
2:C:437:SER:O	2:C:441:LYS:HG3	2.20	0.42
4:d:326:THR:HG22	4:d:344:LYS:HG2	2.02	0.42
1:e:161:HIS:CD2	1:e:163:MET:SD	3.13	0.42
1:e:224:ILE:HG21	1:e:257:ILE:HD11	2.02	0.42
3:F:530:LYS:HE3	3:F:530:LYS:HB3	1.73	0.42
4:f:158:HIS:HA	4:f:161:ARG:HG3	2.01	0.42
2:C:29:ASN:HB2	3:D:246:LEU:H	1.85	0.42
3:D:312:LEU:HD12	3:D:313:LYS:N	2.35	0.42
4:d:229:TYR:O	4:d:234:LYS:N	2.49	0.42
2:E:123:GLN:HG3	2:E:355:LEU:HD21	2.02	0.42
2:E:437:SER:O	2:E:441:LYS:HG3	2.20	0.42
1:c:30:ILE:HD11	1:c:350:LEU:HD11	2.02	0.41
1:c:88:LYS:HB3	1:c:373:PHE:CE1	2.50	0.41
1:c:171:PHE:HB2	1:c:276:PHE:CE1	2.55	0.41
3:D:124:LYS:HB3	3:D:124:LYS:HE2	1.82	0.41
3:D:531:ASP:OD1	3:D:532:HIS:ND1	2.53	0.41
3:F:35:LYS:HE3	3:F:35:LYS:HB2	1.94	0.41
4:f:255:THR:O	4:f:358:GLY:HA2	2.20	0.41
4:f:406:ARG:HG2	4:f:407:PHE:H	1.85	0.41
1:c:276:PHE:CE2	1:c:290:ILE:HG13	2.55	0.41
3:D:284:MET:HE2	3:D:284:MET:HB3	1.97	0.41
4:d:26:ILE:HD12	4:d:26:ILE:O	2.20	0.41
4:d:177:ASP:OD1	4:d:178:GLU:HG2	2.20	0.41
3:F:104:ASN:O	3:F:108:THR:HG23	2.20	0.41
2:C:618:PHE:HA	4:d:321:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:107:THR:HG23	4:d:406:ARG:HA	2.01	0.41
3:D:313:LYS:HE2	3:D:313:LYS:HB3	1.85	0.41
3:F:509:ASN:HB2	3:F:513:SER:OG	2.20	0.41
4:f:224:ARG:O	4:f:228:GLU:N	2.43	0.41
2:C:172:GLU:CD	4:d:258:ILE:HG12	2.46	0.41
2:C:197:LYS:HA	2:C:350:MET:O	2.20	0.41
3:D:282:LEU:HD11	3:D:591:ALA:HB3	2.02	0.41
2:E:580:SER:HB2	3:F:375:MET:HE1	2.03	0.41
1:c:364:VAL:HG22	1:c:375:LYS:HB3	2.02	0.41
2:C:48:THR:O	2:C:190:THR:HG23	2.20	0.41
2:C:82:VAL:HA	2:C:97:VAL:HG12	2.02	0.41
2:C:501:TRP:CH2	3:D:161:ARG:HG3	2.56	0.41
1:e:243:GLN:HA	1:e:246:ILE:HG22	2.02	0.41
4:f:208:LEU:HB2	4:f:209:PRO:HD3	2.01	0.41
3:D:556:HIS:NE2	4:d:403:ASN:HA	2.36	0.41
4:d:179:ILE:H	4:d:179:ILE:HG13	1.66	0.41
1:e:450:THR:HG22	1:e:451:SER:H	1.85	0.41
1:e:450:THR:HG23	1:e:458:SER:O	2.21	0.41
2:E:334:GLU:HG2	2:E:335:ASN:N	2.36	0.41
2:C:166:TYR:OH	2:C:415:GLN:OE1	2.36	0.41
1:e:276:PHE:CD2	1:e:290:ILE:HG13	2.55	0.41
4:f:42:PHE:CE1	4:f:157:SER:HA	2.56	0.41
1:c:236:PHE:CE1	1:c:242:ASN:HB3	2.55	0.41
1:e:37:ILE:O	1:e:40:THR:OG1	2.28	0.41
1:e:139:THR:HA	1:e:302:THR:HG21	2.01	0.41
2:E:408:PHE:HD1	3:F:219:VAL:HG11	1.85	0.41
1:c:122:GLN:O	1:c:343:ILE:HA	2.21	0.41
2:C:439:GLU:O	2:C:442:VAL:HG22	2.21	0.41
3:D:514:LYS:HD3	3:D:514:LYS:HA	1.83	0.41
4:d:20:ILE:HG23	4:d:34:ASP:O	2.20	0.41
2:E:30:LYS:O	2:E:413:PRO:HD2	2.21	0.41
2:E:140:LYS:HE2	2:E:140:LYS:HB3	1.86	0.41
1:c:41:LEU:HD23	1:c:361:THR:HG22	2.03	0.41
2:C:411:LEU:HD22	3:D:242:PHE:CE2	2.56	0.41
3:D:310:ASP:O	3:D:314:ARG:HG2	2.21	0.41
2:C:139:GLU:HG2	2:C:140:LYS:H	1.87	0.40
1:e:40:THR:O	1:e:43:ILE:HG12	2.21	0.40
1:e:77:LEU:HD23	1:e:102:PRO:HA	2.03	0.40
4:f:267:MET:HA	4:f:268:PRO:HD3	1.98	0.40
1:c:183:SER:HB2	1:c:291:ILE:HD11	2.03	0.40
2:C:75:LYS:HG2	2:C:76:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:LEU:HD21	2:C:320:LYS:HD2	2.04	0.40
3:D:311:VAL:HG13	3:D:542:ILE:HD12	2.03	0.40
3:D:522:LEU:O	3:D:529:ILE:HD11	2.21	0.40
1:e:122:GLN:O	1:e:343:ILE:HA	2.21	0.40
2:E:196:VAL:HG13	2:E:352:PHE:HB2	2.03	0.40
1:c:85:LEU:HD13	1:c:94:GLU:HG3	2.02	0.40
1:c:187:PHE:CE2	1:c:253:PHE:HZ	2.39	0.40
2:E:330:MET:HE3	2:E:330:MET:HB2	1.97	0.40
3:F:322:ASN:HB2	3:F:328:VAL:HG11	2.04	0.40
4:f:399:LEU:HD22	4:f:407:PHE:HE1	1.86	0.40
2:C:133:LYS:O	2:C:136:ASP:HB2	2.22	0.40
3:D:283:LEU:O	3:D:374:GLY:HA3	2.21	0.40
4:d:36:ILE:HG13	4:d:37:TYR:HD1	1.86	0.40
4:d:84:ASN:HD22	4:d:84:ASN:HA	1.68	0.40
4:d:181:ASN:HA	4:d:184:ASN:HD21	1.87	0.40
1:e:1:MET:HB3	1:e:2:ILE:H	1.76	0.40
1:e:203:LEU:HB3	1:e:207:ASP:HB2	2.03	0.40
4:f:267:MET:HE3	4:f:267:MET:HB2	1.95	0.40
2:C:24:LEU:HD22	2:C:62:GLU:HG3	2.04	0.40
2:C:416:LEU:HD21	3:D:145:VAL:HG12	2.03	0.40
3:D:133:PHE:O	3:D:137:ILE:HG12	2.22	0.40
3:D:302:LEU:HB2	3:D:346:SER:HB2	2.04	0.40
4:d:83:ILE:HA	4:d:86:ILE:HG22	2.04	0.40
4:d:299:TRP:CH2	4:d:303:ILE:HD11	2.56	0.40
1:e:86:ILE:HB	1:e:93:GLU:HG2	2.04	0.40
2:E:106:THR:HG22	2:E:107:LEU:H	1.87	0.40
3:F:350:CYS:SG	3:F:357:CYS:N	2.92	0.40
3:F:420:ILE:HG13	3:F:467:LEU:HD22	2.02	0.40
4:f:167:THR:HA	4:f:172:LYS:HD2	2.03	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	c	482/496 (97%)	473 (98%)	9 (2%)	0	100	100
1	e	482/496 (97%)	474 (98%)	8 (2%)	0	100	100
2	C	637/665 (96%)	625 (98%)	12 (2%)	0	100	100
2	E	637/665 (96%)	627 (98%)	10 (2%)	0	100	100
3	D	477/631 (76%)	471 (99%)	6 (1%)	0	100	100
3	F	594/631 (94%)	584 (98%)	10 (2%)	0	100	100
4	d	406/448 (91%)	398 (98%)	8 (2%)	0	100	100
4	f	406/448 (91%)	399 (98%)	6 (2%)	1 (0%)	43	71
All	All	4121/4480 (92%)	4051 (98%)	69 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	f	201	ASP

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	c	457/469 (97%)	457 (100%)	0	100	100
1	e	457/469 (97%)	457 (100%)	0	100	100
2	C	587/608 (96%)	585 (100%)	2 (0%)	86	86
2	E	587/608 (96%)	587 (100%)	0	100	100
3	D	445/590 (75%)	445 (100%)	0	100	100
3	F	555/590 (94%)	555 (100%)	0	100	100
4	d	375/409 (92%)	375 (100%)	0	100	100
4	f	375/409 (92%)	375 (100%)	0	100	100
All	All	3838/4152 (92%)	3836 (100%)	2 (0%)	100	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	534[A]	HIS
2	C	534[B]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	13	ASN
1	c	251	ASN
1	c	326	ASN
1	c	371	ASN
2	C	9	ASN
2	C	60	ASN
2	C	215	ASN
2	C	300	ASN
2	C	494	ASN
3	D	40	ASN
3	D	104	ASN
3	D	138	ASN
3	D	143	ASN
3	D	212	ASN
3	D	353	ASN
3	D	553	GLN
4	d	15	ASN
4	d	151	ASN
4	d	180	ASN
4	d	213	ASN
4	d	260	HIS
4	d	377	ASN
4	d	426	ASN
1	e	241	ASN
1	e	280	ASN
1	e	284	GLN
2	E	64	GLN
2	E	89	ASN
2	E	163	ASN
2	E	250	ASN
3	F	418	ASN
3	F	483	ASN
3	F	532	HIS
3	F	553	GLN
4	f	84	ASN
4	f	247	ASN
4	f	252	ASN

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Mol	Chain	Res	Type
4	f	260	HIS
4	f	361	ASN
4	f	377	ASN
4	f	384	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	c	484/496 (97%)	-0.43	0 100 100	57, 129, 227, 365	0
1	e	484/496 (97%)	-0.44	1 (0%) 91 86	109, 173, 251, 319	0
2	C	640/665 (96%)	-0.53	0 100 100	49, 92, 202, 317	1 (0%)
2	E	640/665 (96%)	-0.42	3 (0%) 87 76	94, 151, 214, 279	1 (0%)
3	D	481/631 (76%)	-0.47	0 100 100	54, 112, 194, 261	0
3	F	596/631 (94%)	-0.44	1 (0%) 91 86	121, 175, 272, 329	0
4	d	410/448 (91%)	-0.41	1 (0%) 91 86	71, 179, 259, 367	0
4	f	410/448 (91%)	-0.40	0 100 100	123, 196, 278, 427	0
All	All	4145/4480 (92%)	-0.45	6 (0%) 92 90	49, 152, 250, 427	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	e	246	ILE	2.6
2	E	242	ALA	2.2
3	F	468	PHE	2.2
2	E	523	ILE	2.2
2	E	534[A]	HIS	2.1
4	d	160	LEU	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](#)

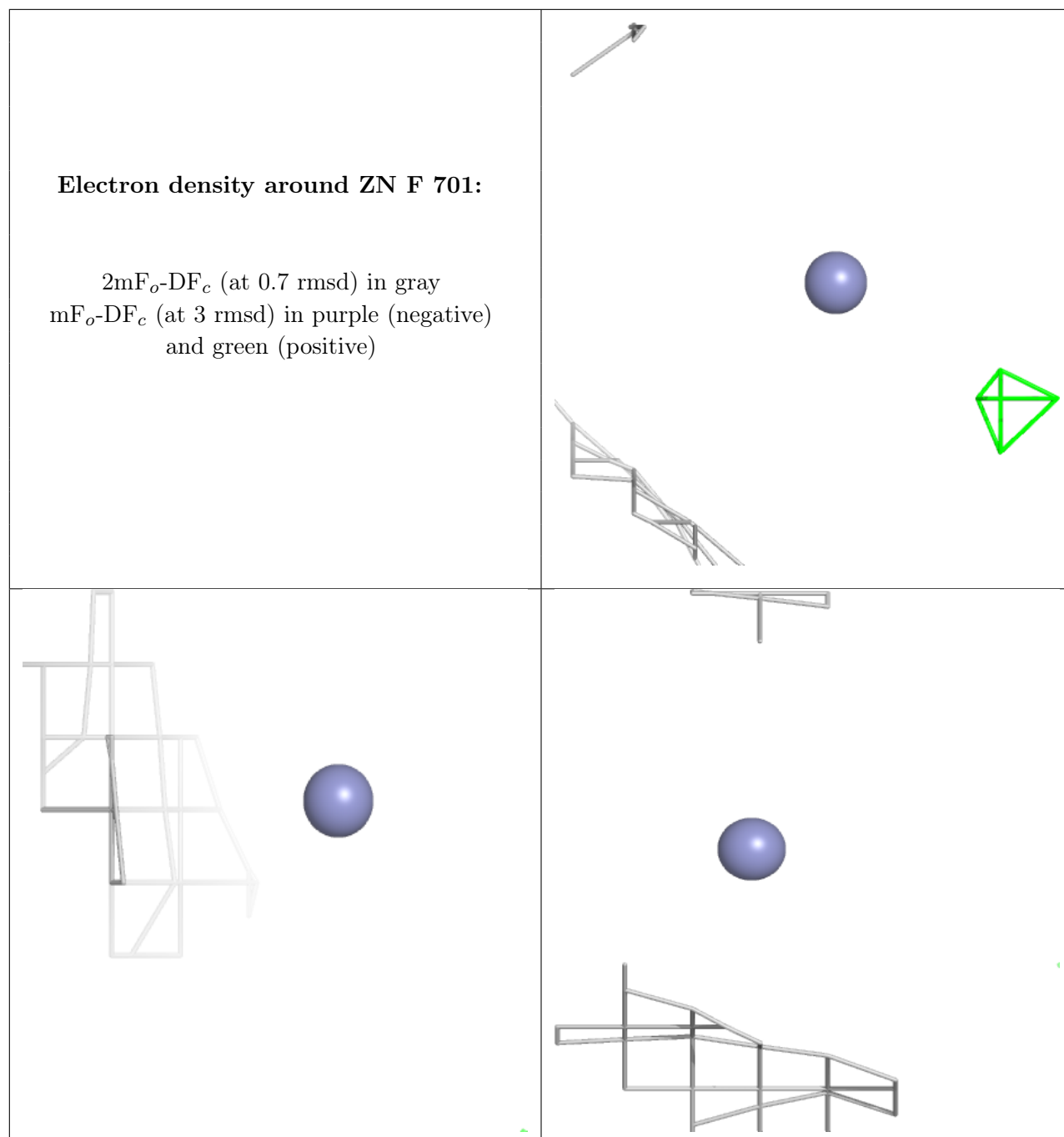
There are no oligosaccharides in this entry.

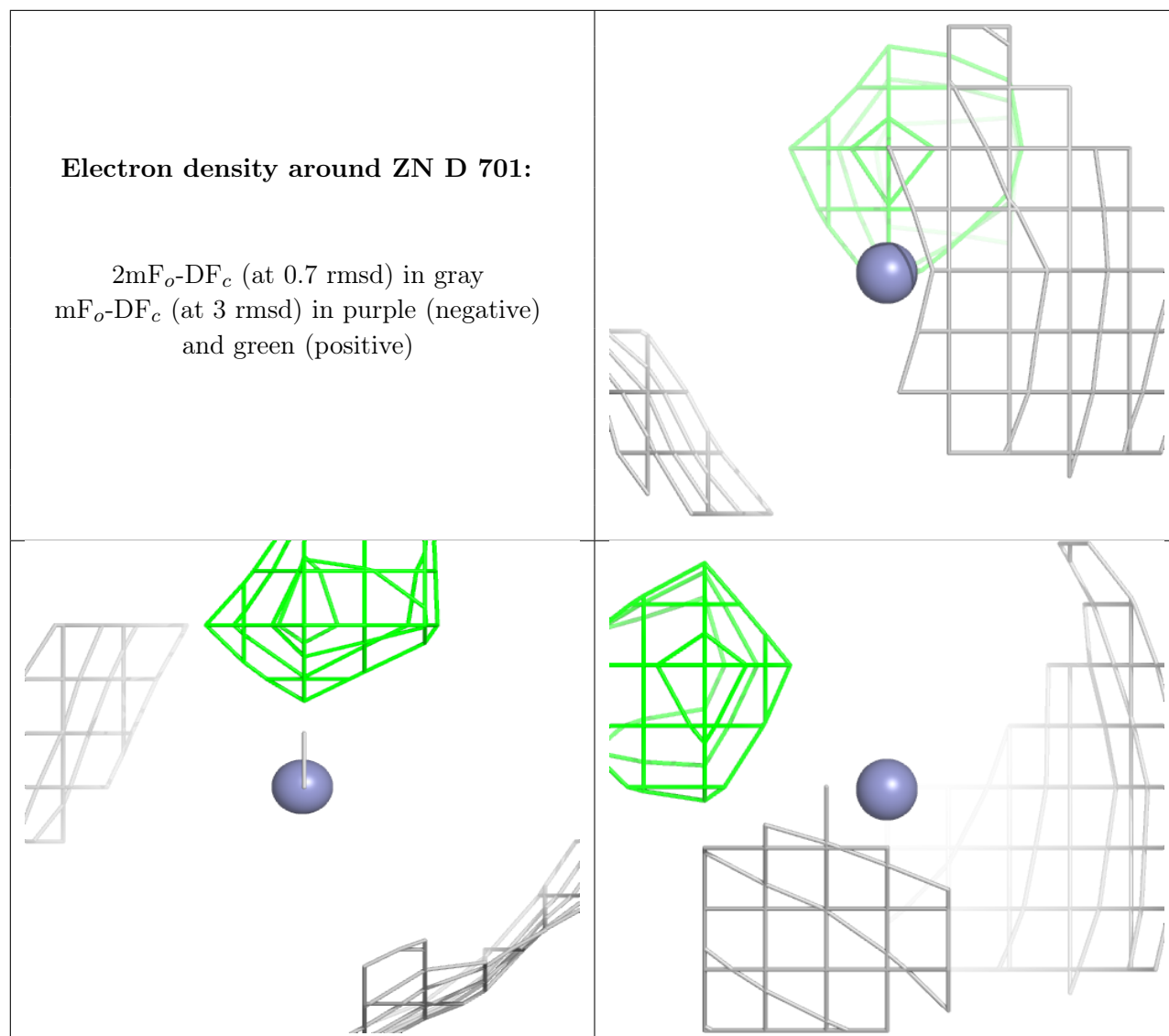
6.4 Ligands

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
5	ZN	F	701	1/1	0.95	0.06	188,188,188,188	0
5	ZN	D	701	1/1	0.99	0.04	135,135,135,135	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.