



Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 05:46 PM GMT

PDB ID : 4LIN
Title : Exploring the atomic structure and conformational flexibility of a 320 angstrom long engineered viral fiber using X-ray crystallography
Authors : Bhardwaj, A.; Cingolani, G.
Deposited on : 2013-07-02
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

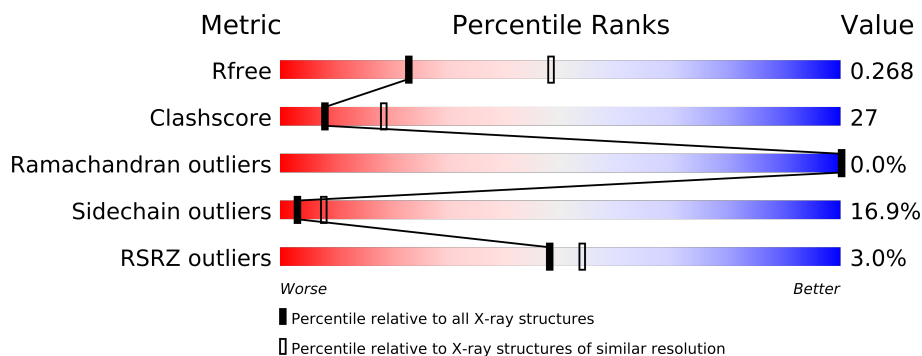
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22714
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	300	
1	B	300	
1	C	300	
1	D	300	
1	E	300	
1	F	300	
1	G	300	
1	H	300	
1	I	300	
1	J	300	
1	K	300	
1	L	300	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CL	I	1301	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26552 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Tail needle protein gp26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	B	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	C	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	D	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	E	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	F	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	G	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	H	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	I	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	J	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	K	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	L	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ca	0	0
			1	1		
2	J	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	E	1	Total 1	Ca 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Cl 1	0	0
3	K	1	Total 1	Cl 1	0	0
3	E	1	Total 1	Cl 1	0	0
3	H	1	Total 1	Cl 1	0	0
3	I	1	Total 1	Cl 1	0	0
3	A	2	Total 2	Cl 2	0	0
3	L	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total 70	O 70	0	0
4	B	81	Total 81	O 81	0	0
4	C	54	Total 54	O 54	0	0
4	D	68	Total 68	O 68	0	0
4	E	61	Total 61	O 61	0	0
4	F	70	Total 70	O 70	0	0
4	G	58	Total 58	O 58	0	0
4	H	54	Total 54	O 54	0	0

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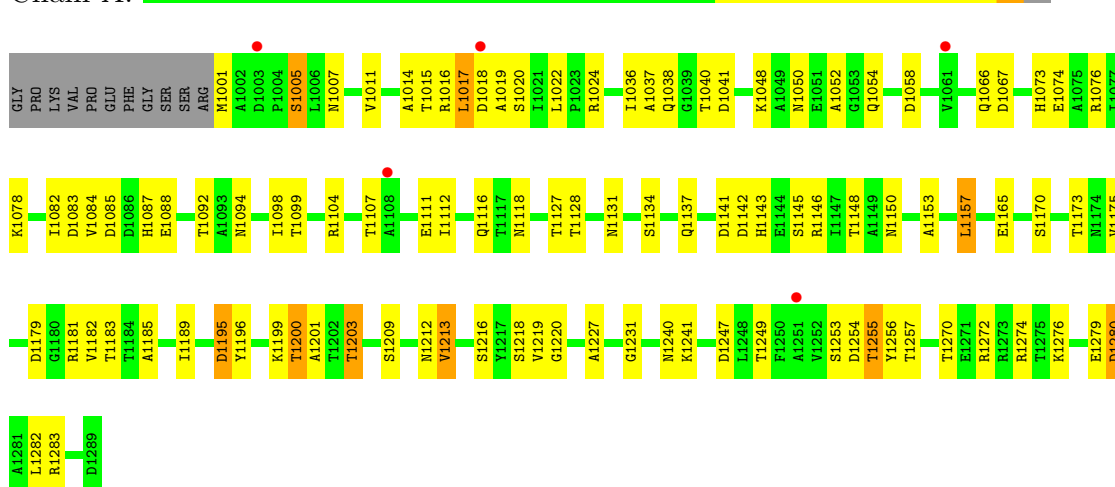
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	61	Total 61	O 61	0	0
4	J	67	Total 67	O 67	0	0
4	K	53	Total 53	O 53	0	0
4	L	67	Total 67	O 67	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

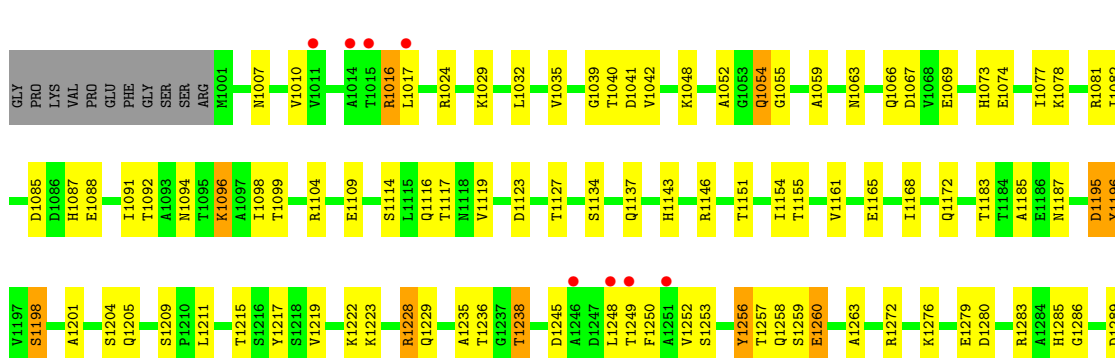
• Molecule 1: Tail needle protein gp26

Chain A:



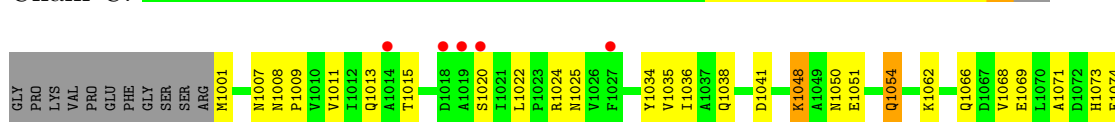
• Molecule 1: Tail needle protein gp26

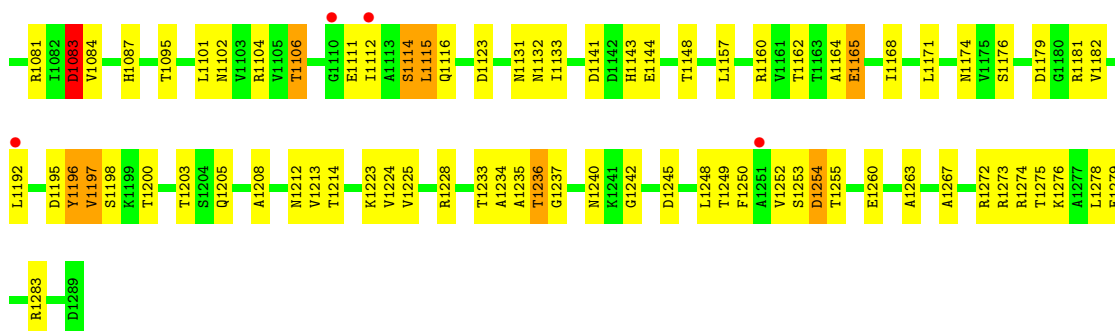
Chain B:



• Molecule 1: Tail needle protein gp26

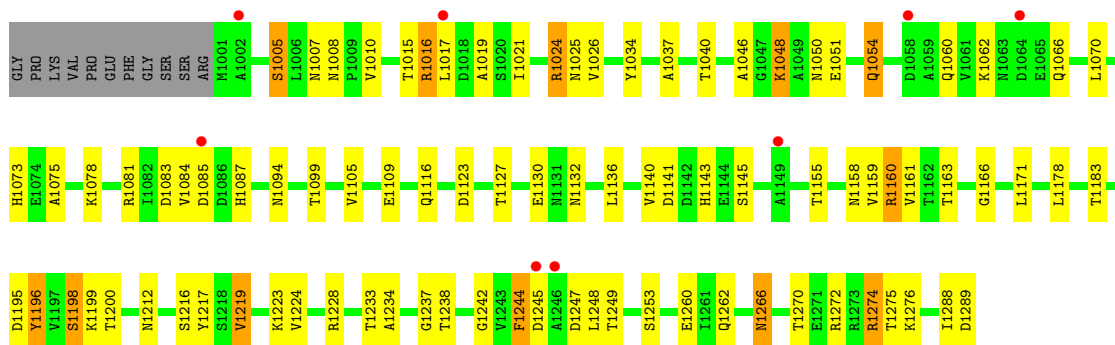
Chain C:





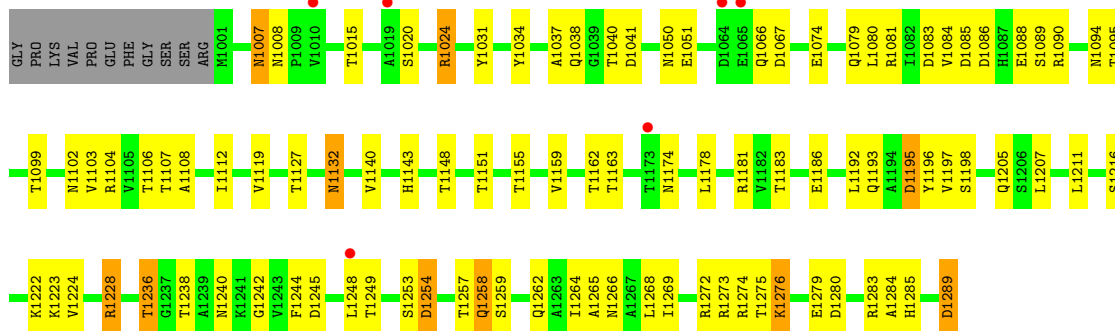
- Molecule 1: Tail needle protein gp26

Chain D:



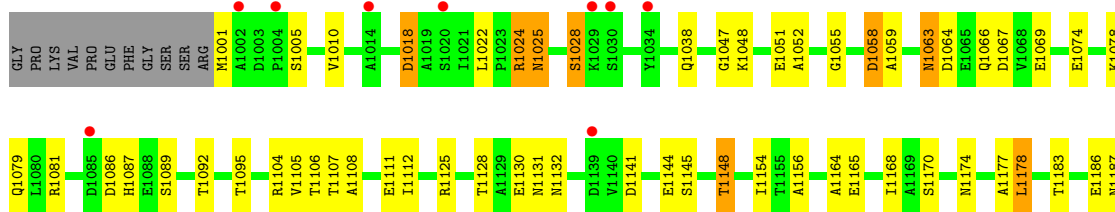
- Molecule 1: Tail needle protein gp26

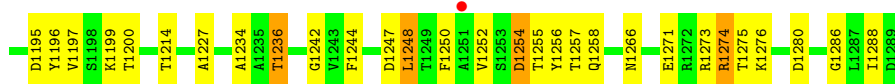
Chain E:



- Molecule 1: Tail needle protein gp26

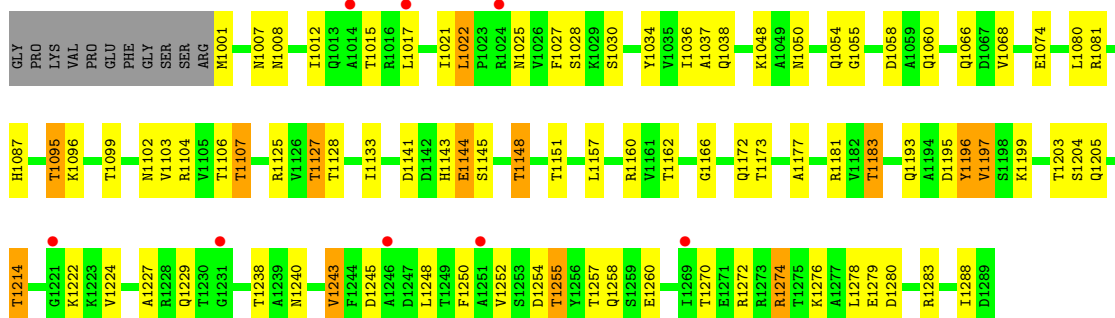
Chain F:





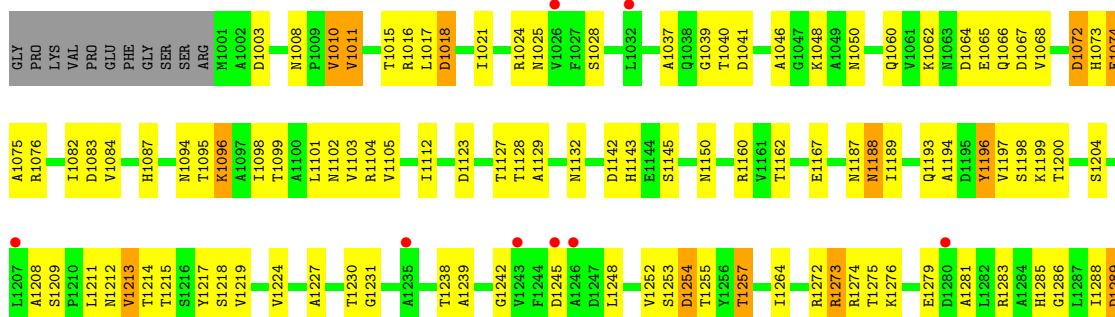
• Molecule 1: Tail needle protein gp26

Chain G:



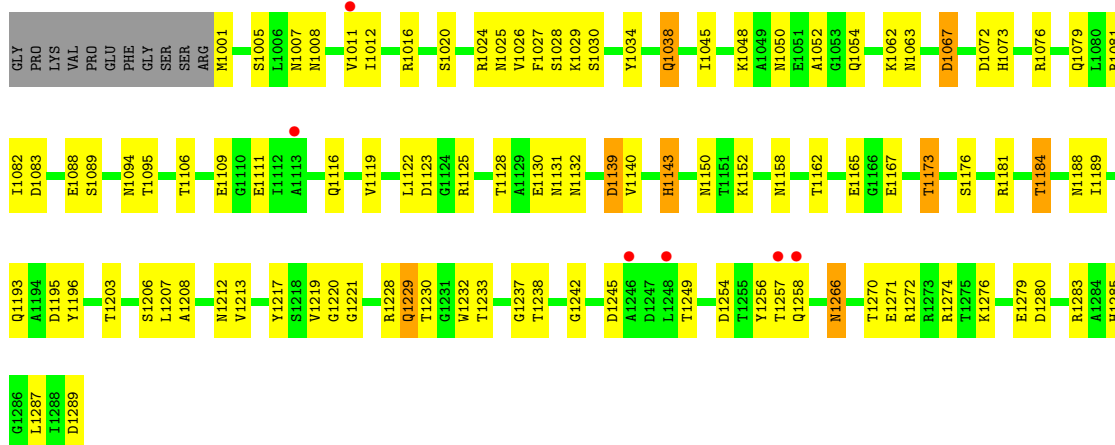
• Molecule 1: Tail needle protein gp26

Chain H:



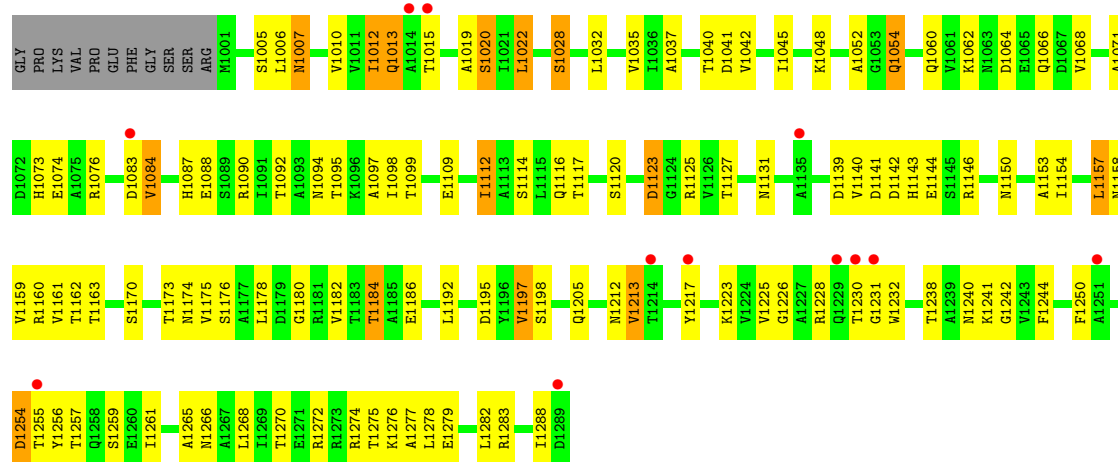
• Molecule 1: Tail needle protein gp26

Chain I:



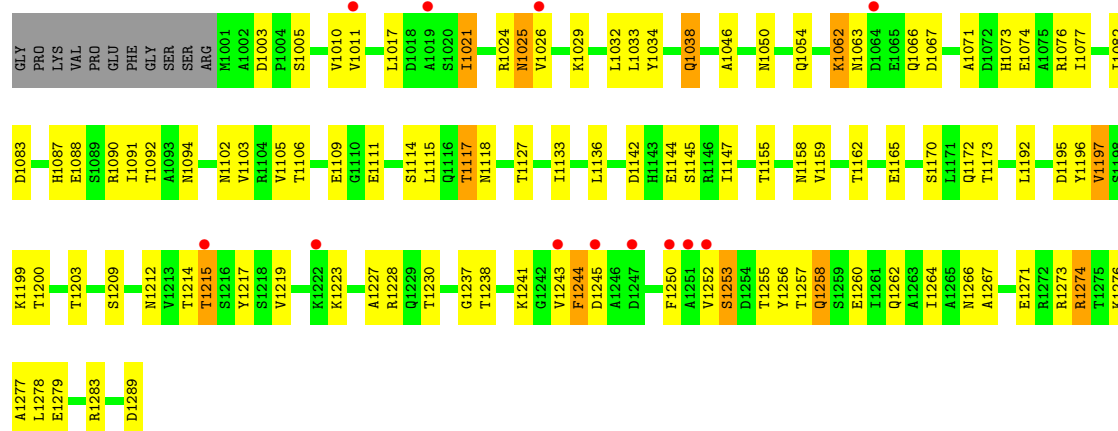
• Molecule 1: Tail needle protein gp26

Chain J:



• Molecule 1: Tail needle protein gp26

Chain K:



• Molecule 1: Tail needle protein gp26

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.69Å 147.93Å 151.01Å 87.94° 90.05° 89.95°	Depositor
Resolution (Å)	14.99 – 2.70 29.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.5 (14.99-2.70) 73.2 (29.92-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.229 , 0.268 0.229 , 0.268	Depositor DCC
R_{free} test set	1835 reflections (2.45%)	DCC
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	1.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 34.8	EDS
Estimated twinning fraction	0.480 for h,-k,-l 0.000 for h,-l,k 0.000 for h,l,-k 0.429 for h,-k,-l 0.000 for -h,k,-l 0.000 for -h,-k,l 0.000 for -h,-l,-k 0.000 for -h,l,k	Xtriage
Reported twinning fraction	0.480 for h,-k,-l	Depositor
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 73916 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	26552	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.27	0/2166	0.48	0/2950
1	B	0.26	0/2166	0.51	1/2950 (0.0%)
1	C	0.30	0/2166	0.55	1/2950 (0.0%)
1	D	0.27	0/2166	0.48	0/2950
1	E	0.26	0/2166	0.48	0/2950
1	F	0.26	0/2166	0.52	1/2950 (0.0%)
1	G	0.28	0/2166	0.51	0/2950
1	H	0.30	0/2166	0.52	0/2950
1	I	0.29	0/2166	0.49	0/2950
1	J	0.27	0/2166	0.51	0/2950
1	K	0.27	0/2166	0.52	0/2950
1	L	0.28	0/2166	0.52	0/2950
All	All	0.28	0/25992	0.51	3/35400 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1248	LEU	CA-CB-CG	5.45	127.83	115.30
1	F	1248	LEU	CA-CB-CG	5.08	126.99	115.30
1	C	1083	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2148	0	0	68	1
1	B	2148	0	0	65	0
1	C	2148	0	0	68	0
1	D	2148	0	0	67	0
1	E	2148	0	0	65	1
1	F	2148	0	0	63	1
1	G	2148	0	0	65	0
1	H	2148	0	0	66	0
1	I	2148	0	0	74	1
1	J	2148	0	0	81	2
1	K	2148	0	0	70	1
1	L	2148	0	0	70	0
2	A	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	J	1	0	0	0	0
3	A	2	0	0	3	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	2	0
3	I	1	0	0	2	0
3	K	1	0	0	1	0
3	L	1	0	0	2	0
4	A	70	0	0	31	0
4	B	81	0	0	28	2
4	C	54	0	0	22	0
4	D	68	0	0	35	2
4	E	61	0	0	27	0
4	F	70	0	0	26	2
4	G	58	0	0	30	0
4	H	54	0	0	24	0
4	I	61	0	0	30	0
4	J	67	0	0	21	0
4	K	53	0	0	19	0
4	L	67	0	0	27	1
All	All	26552	0	0	690	7

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (690) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:1087:HIS:CD2	4:H:1454:HOH:O	1.98	1.12
1:K:1054:GLN:NE2	4:K:1440:HOH:O	1.82	1.11
1:J:1265:ALA:CB	1:K:1250:PHE:CE2	2.34	1.08
1:L:1187:ASN:ND2	4:L:1441:HOH:O	1.87	1.07
1:A:1212:ASN:ND2	4:A:1439:HOH:O	1.85	1.06
1:K:1273:ARG:NH1	4:K:1401:HOH:O	1.89	1.05
1:J:1197:VAL:O	1:L:1197:VAL:CG2	2.05	1.05
1:K:1172:GLN:NE2	4:K:1415:HOH:O	1.90	1.04
1:H:1096:LYS:NZ	4:H:1433:HOH:O	1.92	1.03
1:F:1266:ASN:ND2	4:F:1312:HOH:O	1.92	1.03
1:E:1079:GLN:NE2	4:E:1445:HOH:O	1.93	0.99
1:E:1236:THR:OG1	4:E:1402:HOH:O	1.81	0.97
1:C:1143:HIS:ND1	4:C:1336:HOH:O	1.96	0.97
1:I:1116:GLN:NE2	4:I:1414:HOH:O	1.95	0.97
1:B:1109:GLU:OE1	4:B:1358:HOH:O	1.83	0.96
1:A:1279:GLU:OE1	4:A:1458:HOH:O	1.82	0.96
1:B:1024:ARG:O	4:B:1354:HOH:O	1.84	0.95
1:B:1134:SER:N	4:B:1317:HOH:O	1.98	0.94
1:A:1118:ASN:ND2	4:A:1437:HOH:O	2.00	0.94
1:G:1238:THR:O	4:G:1406:HOH:O	1.84	0.94
1:L:1134:SER:OG	4:L:1407:HOH:O	1.84	0.94
1:E:1284:ALA:O	4:E:1451:HOH:O	1.85	0.94
1:E:1280:ASP:OD1	4:E:1453:HOH:O	1.86	0.93
1:K:1250:PHE:CE1	1:K:1264:ILE:CA	2.53	0.92
1:E:1223:LYS:NZ	4:E:1436:HOH:O	2.02	0.92
1:B:1172:GLN:O	4:B:1334:HOH:O	1.87	0.92
1:L:1134:SER:O	4:L:1437:HOH:O	1.87	0.92
1:L:1120:SER:OG	4:L:1414:HOH:O	1.88	0.91
1:K:1258:GLN:NE2	4:K:1429:HOH:O	2.03	0.91
1:C:1102:ASN:ND2	4:C:1349:HOH:O	2.04	0.91
1:D:1166:GLY:O	4:D:1432:HOH:O	1.88	0.91
1:L:1150:ASN:ND2	3:L:1301:CL:CL	2.41	0.91
1:J:1150:ASN:ND2	3:L:1301:CL:CL	2.40	0.90
1:D:1228:ARG:NH1	4:D:1430:HOH:O	2.04	0.90
1:D:1237:GLY:O	4:D:1451:HOH:O	1.89	0.90
1:B:1096:LYS:NZ	4:B:1324:HOH:O	2.04	0.90
1:J:1005:SER:OG	4:J:1455:HOH:O	1.88	0.90
1:F:1227:ALA:O	4:F:1316:HOH:O	1.88	0.90
1:B:1134:SER:OG	4:B:1317:HOH:O	1.90	0.90
1:B:1016:ARG:N	4:B:1367:HOH:O	2.04	0.90
1:A:1150:ASN:ND2	3:A:1302:CL:CL	2.42	0.90
1:K:1071:ALA:O	4:K:1453:HOH:O	1.90	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:1289:ASP:OD2	4:K:1428:HOH:O	1.90	0.89
1:G:1177:ALA:O	4:G:1451:HOH:O	1.91	0.89
1:A:1203:THR:OG1	4:A:1427:HOH:O	1.91	0.88
1:C:1007:ASN:OD1	1:C:1054:GLN:NE2	2.06	0.88
1:G:1222:LYS:NZ	4:G:1410:HOH:O	2.06	0.88
1:C:1001:MET:O	4:C:1313:HOH:O	1.91	0.88
1:E:1244:PHE:N	4:E:1410:HOH:O	2.06	0.87
1:J:1142:ASP:OD2	4:J:1410:HOH:O	1.93	0.87
1:J:1153:ALA:O	4:J:1416:HOH:O	1.92	0.87
1:G:1193:GLN:O	4:G:1449:HOH:O	1.93	0.87
1:K:1010:VAL:O	4:K:1441:HOH:O	1.93	0.86
1:F:1258:GLN:NE2	4:F:1334:HOH:O	2.06	0.86
1:H:1102:ASN:N	4:H:1432:HOH:O	2.08	0.86
1:D:1099:THR:OG1	4:D:1450:HOH:O	1.91	0.86
1:F:1131:ASN:ND2	4:F:1315:HOH:O	2.09	0.86
1:K:1087:HIS:NE2	1:L:1088:GLU:OE2	2.08	0.86
3:H:1301:CL:CL	1:I:1094:ASN:ND2	2.46	0.86
1:E:1276:LYS:N	4:E:1420:HOH:O	2.09	0.86
1:J:1265:ALA:CB	1:K:1250:PHE:CD2	2.59	0.86
1:J:1073:HIS:ND1	4:J:1417:HOH:O	2.09	0.86
1:F:1001:MET:O	4:F:1335:HOH:O	1.93	0.86
1:C:1009:PRO:O	4:C:1306:HOH:O	1.93	0.85
1:J:1048:LYS:NZ	1:K:1050:ASN:OD1	2.10	0.85
1:G:1050:ASN:ND2	4:G:1432:HOH:O	2.10	0.85
1:A:1001:MET:O	4:A:1449:HOH:O	1.94	0.85
1:C:1234:ALA:O	4:C:1301:HOH:O	1.95	0.84
1:I:1203:THR:O	4:I:1457:HOH:O	1.95	0.84
1:B:1069:GLU:OE2	4:B:1308:HOH:O	1.94	0.84
1:K:1223:LYS:O	1:L:1228:ARG:NH2	2.10	0.84
1:L:1186:GLU:OE2	4:L:1444:HOH:O	1.95	0.84
1:L:1020:SER:OG	4:L:1454:HOH:O	1.96	0.84
1:L:1100:ALA:N	4:L:1405:HOH:O	2.11	0.84
1:D:1238:THR:N	4:D:1431:HOH:O	2.10	0.83
1:F:1106:THR:N	4:F:1367:HOH:O	2.09	0.83
1:H:1028:SER:OG	4:H:1425:HOH:O	1.94	0.83
1:K:1250:PHE:CD1	1:K:1264:ILE:CG1	2.61	0.83
1:D:1116:GLN:O	4:D:1437:HOH:O	1.96	0.83
1:F:1165:GLU:OE1	4:F:1323:HOH:O	1.94	0.83
1:L:1196:TYR:CE1	1:L:1198:SER:CB	2.61	0.83
1:G:1214:THR:OG1	4:G:1438:HOH:O	1.96	0.82
1:J:1217:TYR:CD2	1:J:1225:VAL:CB	2.62	0.82
1:A:1038:GLN:NE2	4:A:1416:HOH:O	2.12	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1183:THR:N	4:A:1445:HOH:O	2.12	0.82
1:I:1079:GLN:OE1	4:I:1425:HOH:O	1.96	0.82
1:E:1276:LYS:NZ	4:E:1438:HOH:O	2.11	0.82
1:J:1232:TRP:O	4:J:1401:HOH:O	1.96	0.82
4:E:1402:HOH:O	1:F:1244:PHE:O	1.97	0.81
1:G:1238:THR:N	4:G:1406:HOH:O	2.13	0.81
1:G:1145:SER:N	4:G:1408:HOH:O	2.13	0.81
1:A:1274:ARG:NH2	4:A:1402:HOH:O	2.11	0.81
1:E:1099:THR:OG1	4:E:1419:HOH:O	1.96	0.81
1:A:1050:ASN:OD1	1:C:1048:LYS:NZ	2.13	0.81
1:J:1071:ALA:O	4:J:1441:HOH:O	1.97	0.81
1:B:1024:ARG:N	4:B:1329:HOH:O	2.13	0.81
1:H:1160:ARG:NH1	1:I:1158:ASN:OD1	2.14	0.81
1:H:1242:GLY:O	1:H:1274:ARG:NH1	2.14	0.80
1:D:1270:THR:OG1	4:D:1407:HOH:O	1.99	0.80
1:G:1143:HIS:ND1	4:G:1434:HOH:O	2.13	0.80
1:L:1247:ASP:OD2	4:L:1467:HOH:O	1.99	0.80
1:A:1017:LEU:O	4:A:1440:HOH:O	2.00	0.80
1:G:1258:GLN:NE2	1:H:1253:SER:O	2.14	0.80
1:I:1208:ALA:O	4:I:1402:HOH:O	2.00	0.79
1:G:1166:GLY:N	4:G:1457:HOH:O	2.15	0.79
1:E:1143:HIS:ND1	4:E:1439:HOH:O	2.16	0.79
1:A:1019:ALA:O	4:A:1469:HOH:O	2.01	0.79
1:E:1066:GLN:NE2	1:F:1067:ASP:OD1	2.16	0.79
1:H:1039:GLY:O	4:H:1405:HOH:O	2.00	0.79
1:D:1008:ASN:O	1:F:1048:LYS:NZ	2.16	0.78
1:F:1275:THR:OG1	4:F:1360:HOH:O	2.00	0.78
1:G:1245:ASP:O	1:I:1272:ARG:NH1	2.16	0.78
1:B:1073:HIS:ND1	4:B:1336:HOH:O	2.16	0.78
1:E:1269:ILE:N	4:E:1432:HOH:O	2.16	0.78
1:H:1073:HIS:ND1	4:H:1427:HOH:O	2.16	0.78
1:G:1162:THR:O	4:G:1457:HOH:O	2.02	0.78
1:A:1231:GLY:O	4:A:1409:HOH:O	2.02	0.78
1:I:1072:ASP:OD2	4:I:1418:HOH:O	2.01	0.77
1:I:1206:SER:O	4:I:1410:HOH:O	2.01	0.77
1:H:1227:ALA:O	1:I:1285:HIS:NE2	2.17	0.77
1:K:1279:GLU:OE2	1:K:1283:ARG:NH2	2.17	0.77
1:E:1242:GLY:O	1:E:1274:ARG:NH1	2.18	0.77
1:I:1130:GLU:OE2	4:I:1445:HOH:O	2.01	0.77
1:I:1220:GLY:N	4:I:1447:HOH:O	2.16	0.77
1:A:1066:GLN:NE2	1:B:1067:ASP:OD1	2.18	0.77
1:D:1010:VAL:O	4:D:1454:HOH:O	2.01	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1026:VAL:O	4:D:1464:HOH:O	2.01	0.76
1:C:1131:ASN:ND2	4:C:1334:HOH:O	2.18	0.76
1:H:1024:ARG:NH1	4:H:1441:HOH:O	2.18	0.76
1:I:1048:LYS:NZ	4:I:1440:HOH:O	2.16	0.76
1:E:1031:TYR:OH	4:E:1425:HOH:O	2.04	0.76
3:A:1303:CL:CL	1:B:1094:ASN:ND2	2.56	0.76
1:K:1011:VAL:O	4:K:1403:HOH:O	2.05	0.75
1:F:1288:ILE:O	4:F:1311:HOH:O	2.03	0.75
1:A:1005:SER:OG	4:A:1422:HOH:O	2.04	0.75
1:K:1094:ASN:ND2	3:K:1301:CL:CL	2.57	0.75
1:D:1237:GLY:O	1:D:1276:LYS:NZ	2.20	0.75
1:L:1196:TYR:O	1:L:1197:VAL:CG2	2.35	0.75
1:I:1188:ASN:OD1	4:I:1427:HOH:O	2.05	0.75
1:L:1008:ASN:ND2	4:L:1456:HOH:O	2.19	0.75
1:E:1283:ARG:NH1	1:E:1289:ASP:OD1	2.20	0.74
1:H:1285:HIS:N	4:H:1419:HOH:O	2.21	0.74
1:G:1205:GLN:O	4:G:1402:HOH:O	2.03	0.74
1:E:1272:ARG:NH2	1:F:1247:ASP:OD2	2.20	0.74
1:K:1117:THR:N	4:K:1439:HOH:O	2.20	0.74
1:B:1263:ALA:O	4:B:1311:HOH:O	2.05	0.74
1:H:1239:ALA:O	4:H:1430:HOH:O	2.05	0.74
1:D:1260:GLU:OE2	4:D:1459:HOH:O	2.05	0.74
1:I:1229:GLN:OE1	1:I:1232:TRP:NE1	2.21	0.73
1:F:1051:GLU:OE1	4:F:1354:HOH:O	2.05	0.73
1:J:1098:ILE:N	4:J:1439:HOH:O	2.21	0.73
1:G:1229:GLN:NE2	4:H:1419:HOH:O	2.21	0.73
1:B:1185:ALA:O	4:B:1339:HOH:O	2.06	0.73
1:K:1158:ASN:OD1	4:K:1448:HOH:O	2.07	0.73
1:A:1272:ARG:NH2	4:A:1447:HOH:O	2.20	0.73
1:L:1016:ARG:NH2	4:L:1436:HOH:O	2.20	0.73
1:G:1103:VAL:O	1:G:1107:THR:OG1	2.07	0.73
1:E:1272:ARG:O	4:E:1420:HOH:O	2.06	0.73
1:D:1130:GLU:O	4:D:1468:HOH:O	2.06	0.73
1:G:1199:LYS:NZ	1:I:1196:TYR:O	2.21	0.73
1:L:1196:TYR:O	4:L:1461:HOH:O	2.06	0.72
1:C:1116:GLN:O	4:C:1320:HOH:O	2.05	0.72
1:J:1146:ARG:NH2	1:K:1144:GLU:OE1	2.23	0.72
1:K:1197:VAL:O	4:K:1430:HOH:O	2.06	0.72
1:B:1183:THR:O	1:B:1187:ASN:ND2	2.23	0.72
1:J:1288:ILE:O	4:J:1412:HOH:O	2.07	0.72
1:J:1097:ALA:N	4:J:1439:HOH:O	2.22	0.72
1:L:1240:ASN:O	4:L:1459:HOH:O	2.08	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1048:LYS:O	1:A:1052:ALA:N	2.23	0.72
1:K:1258:GLN:O	1:K:1262:GLN:NE2	2.23	0.72
1:G:1081:ARG:NH2	4:G:1421:HOH:O	2.23	0.72
1:D:1087:HIS:ND1	4:D:1448:HOH:O	2.23	0.71
1:J:1109:GLU:OE2	4:J:1459:HOH:O	2.07	0.71
1:G:1141:ASP:O	4:G:1408:HOH:O	2.08	0.71
1:J:1073:HIS:NE2	1:K:1074:GLU:OE1	2.24	0.71
1:J:1240:ASN:O	1:J:1274:ARG:NH1	2.24	0.71
1:H:1275:THR:OG1	1:I:1271:GLU:OE2	2.08	0.71
1:L:1210:PRO:O	4:L:1465:HOH:O	2.06	0.71
1:B:1116:GLN:NE2	4:B:1309:HOH:O	2.24	0.71
1:B:1096:LYS:O	4:B:1312:HOH:O	2.07	0.71
1:L:1131:ASN:ND2	4:L:1448:HOH:O	2.24	0.71
1:A:1280:ASP:OD1	4:A:1428:HOH:O	2.08	0.71
1:E:1264:ILE:O	4:E:1401:HOH:O	2.09	0.71
1:C:1071:ALA:O	4:C:1315:HOH:O	2.09	0.70
1:B:1048:LYS:NZ	1:C:1008:ASN:O	2.24	0.70
1:E:1228:ARG:O	4:E:1408:HOH:O	2.08	0.70
1:I:1242:GLY:O	1:I:1274:ARG:NH1	2.24	0.70
1:H:1024:ARG:N	4:H:1407:HOH:O	2.23	0.70
1:G:1081:ARG:NH1	1:I:1083:ASP:OD2	2.24	0.70
1:E:1265:ALA:O	4:E:1432:HOH:O	2.07	0.70
4:D:1448:HOH:O	1:F:1087:HIS:ND1	2.24	0.70
1:D:1083:ASP:O	4:D:1449:HOH:O	2.10	0.70
1:C:1208:ALA:O	4:C:1318:HOH:O	2.10	0.70
1:K:1029:LYS:NZ	4:K:1405:HOH:O	2.25	0.70
1:J:1226:GLY:O	4:J:1407:HOH:O	2.09	0.70
1:I:1150:ASN:ND2	3:I:1301:CL:CL	2.62	0.70
1:D:1073:HIS:ND1	4:D:1447:HOH:O	2.24	0.70
1:C:1240:ASN:O	1:C:1274:ARG:NH1	2.25	0.70
1:D:1253:SER:O	1:F:1256:TYR:OH	2.10	0.69
1:F:1174:ASN:O	1:F:1178:LEU:N	2.25	0.69
1:L:1275:THR:OG1	4:L:1415:HOH:O	2.11	0.69
1:L:1096:LYS:O	4:L:1405:HOH:O	2.09	0.69
1:H:1046:ALA:O	1:H:1050:ASN:ND2	2.26	0.69
1:D:1219:VAL:O	4:D:1402:HOH:O	2.09	0.69
1:H:1075:ALA:N	4:H:1431:HOH:O	2.25	0.69
1:D:1132:ASN:ND2	4:D:1423:HOH:O	2.24	0.69
1:H:1094:ASN:ND2	3:H:1301:CL:CL	2.63	0.69
1:G:1066:GLN:NE2	1:H:1067:ASP:OD1	2.24	0.69
1:E:1037:ALA:O	1:E:1041:ASP:N	2.25	0.69
1:F:1064:ASP:OD2	4:F:1353:HOH:O	2.10	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1234:ALA:O	4:D:1429:HOH:O	2.10	0.69
1:J:1094:ASN:O	4:J:1439:HOH:O	2.11	0.69
1:B:1143:HIS:NE2	1:C:1144:GLU:OE1	2.25	0.68
1:G:1048:LYS:NZ	1:H:1008:ASN:O	2.26	0.68
1:C:1197:VAL:N	4:C:1304:HOH:O	2.26	0.68
1:E:1020:SER:O	4:E:1429:HOH:O	2.10	0.68
1:B:1016:ARG:NH2	1:B:1039:GLY:O	2.27	0.68
1:E:1193:GLN:NE2	4:E:1414:HOH:O	2.26	0.68
1:B:1238:THR:OG1	4:B:1301:HOH:O	2.11	0.68
1:L:1007:ASN:OD1	1:L:1054:GLN:NE2	2.26	0.68
1:J:1268:LEU:CD2	1:K:1250:PHE:CZ	2.76	0.68
1:J:1064:ASP:OD1	1:L:1062:LYS:NZ	2.27	0.68
1:D:1262:GLN:OE1	4:D:1439:HOH:O	2.09	0.68
1:D:1075:ALA:N	4:D:1467:HOH:O	2.25	0.68
4:D:1449:HOH:O	1:E:1088:GLU:OE2	2.11	0.67
1:G:1195:ASP:OD2	1:H:1196:TYR:OH	2.11	0.67
1:B:1280:ASP:OD2	4:B:1342:HOH:O	2.11	0.67
1:L:1135:ALA:O	4:L:1458:HOH:O	2.12	0.67
1:A:1083:ASP:OD2	1:B:1081:ARG:NH2	2.27	0.67
1:B:1109:GLU:OE2	4:B:1343:HOH:O	2.11	0.67
1:K:1062:LYS:O	1:K:1066:GLN:N	2.27	0.67
1:I:1082:ILE:O	4:I:1417:HOH:O	2.12	0.67
1:B:1007:ASN:OD1	1:B:1054:GLN:NE2	2.27	0.67
1:L:1196:TYR:C	1:L:1197:VAL:CG2	2.63	0.67
1:D:1048:LYS:NZ	1:E:1008:ASN:O	2.28	0.67
4:J:1459:HOH:O	1:L:1104:ARG:O	2.12	0.67
1:G:1007:ASN:OD1	1:G:1054:GLN:NE2	2.28	0.67
1:A:1201:ALA:N	4:A:1403:HOH:O	2.28	0.67
1:F:1089:SER:OG	4:F:1361:HOH:O	2.12	0.67
4:A:1402:HOH:O	1:C:1279:GLU:OE2	2.13	0.66
1:I:1026:VAL:O	4:I:1459:HOH:O	2.13	0.66
1:F:1028:SER:N	4:F:1370:HOH:O	2.27	0.66
1:C:1102:ASN:O	1:C:1106:THR:OG1	2.14	0.66
1:B:1252:VAL:O	4:B:1333:HOH:O	2.14	0.66
1:J:1275:THR:OG1	4:L:1415:HOH:O	2.13	0.66
1:I:1280:ASP:OD2	4:I:1434:HOH:O	2.13	0.66
1:A:1283:ARG:NH1	4:A:1411:HOH:O	2.28	0.66
1:D:1066:GLN:OE1	1:F:1066:GLN:NE2	2.29	0.66
1:L:1262:GLN:O	1:L:1266:ASN:N	2.29	0.66
1:B:1228:ARG:NE	1:B:1286:GLY:O	2.29	0.66
4:A:1402:HOH:O	1:C:1233:THR:O	2.13	0.66
1:B:1223:LYS:NZ	4:B:1332:HOH:O	2.28	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:1130:GLU:OE1	4:F:1326:HOH:O	2.13	0.66
1:G:1199:LYS:N	1:I:1195:ASP:O	2.28	0.66
1:D:1247:ASP:OD2	1:F:1273:ARG:NE	2.28	0.66
1:J:1060:GLN:NE2	1:L:1055:GLY:O	2.28	0.66
1:H:1048:LYS:NZ	1:I:1050:ASN:OD1	2.29	0.65
1:J:1238:THR:O	1:J:1276:LYS:NZ	2.29	0.65
1:I:1173:THR:OG1	4:I:1426:HOH:O	2.14	0.65
1:J:1198:SER:O	1:J:1205:GLN:NE2	2.29	0.65
1:E:1258:GLN:NE2	4:E:1431:HOH:O	2.30	0.65
1:L:1155:THR:OG1	4:L:1432:HOH:O	2.14	0.65
1:D:1196:TYR:OH	1:F:1195:ASP:OD2	2.14	0.65
1:H:1098:ILE:O	4:H:1432:HOH:O	2.13	0.65
1:L:1228:ARG:NE	1:L:1286:GLY:O	2.29	0.65
1:J:1146:ARG:NH1	4:J:1411:HOH:O	2.28	0.65
1:I:1024:ARG:O	4:I:1446:HOH:O	2.13	0.65
1:G:1172:GLN:OE1	4:G:1407:HOH:O	2.15	0.65
1:E:1195:ASP:O	1:F:1199:LYS:NZ	2.29	0.65
1:A:1240:ASN:ND2	4:A:1425:HOH:O	2.28	0.65
1:E:1107:THR:O	4:E:1441:HOH:O	2.15	0.65
1:I:1279:GLU:OE2	1:I:1283:ARG:NH2	2.30	0.65
1:H:1254:ASP:N	1:H:1254:ASP:OD1	2.30	0.65
1:B:1137:GLN:NE2	4:B:1305:HOH:O	2.29	0.65
1:L:1074:GLU:OE2	1:L:1078:LYS:NZ	2.29	0.65
1:B:1256:TYR:OH	1:C:1253:SER:O	2.15	0.65
1:G:1104:ARG:NH1	4:G:1431:HOH:O	2.30	0.65
1:J:1074:GLU:OE1	1:L:1073:HIS:NE2	2.30	0.65
1:D:1046:ALA:O	1:D:1050:ASN:ND2	2.30	0.65
1:G:1243:VAL:N	4:G:1409:HOH:O	2.28	0.65
1:C:1165:GLU:OE2	4:C:1317:HOH:O	2.14	0.64
1:H:1289:ASP:OD1	1:H:1289:ASP:N	2.29	0.64
1:H:1196:TYR:O	4:H:1409:HOH:O	2.15	0.64
1:G:1160:ARG:NH2	1:H:1162:THR:OG1	2.30	0.64
1:E:1198:SER:O	1:E:1205:GLN:NE2	2.30	0.64
1:J:1090:ARG:NH2	1:K:1092:THR:OG1	2.30	0.64
1:F:1144:GLU:O	1:F:1148:THR:OG1	2.16	0.64
1:B:1073:HIS:NE2	1:C:1074:GLU:OE1	2.31	0.64
1:E:1132:ASN:ND2	4:E:1411:HOH:O	2.30	0.64
1:A:1209:SER:OG	1:B:1205:GLN:OE1	2.16	0.64
1:L:1260:GLU:O	4:L:1423:HOH:O	2.15	0.64
1:E:1083:ASP:OD2	1:F:1081:ARG:NH2	2.31	0.64
1:G:1196:TYR:O	4:G:1417:HOH:O	2.14	0.64
1:E:1236:THR:OG1	1:F:1244:PHE:O	2.15	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:1008:ASN:O	1:I:1048:LYS:NZ	2.32	0.63
1:J:1275:THR:OG1	1:K:1271:GLU:OE2	2.17	0.63
1:C:1112:ILE:O	1:C:1116:GLN:N	2.31	0.63
1:D:1019:ALA:O	1:D:1024:ARG:NH2	2.32	0.63
1:K:1083:ASP:OD2	1:L:1081:ARG:NH2	2.32	0.63
1:J:1162:THR:OG1	1:L:1160:ARG:NH2	2.31	0.63
1:A:1067:ASP:OD1	1:C:1066:GLN:NE2	2.31	0.63
1:D:1073:HIS:NE2	1:E:1074:GLU:OE1	2.31	0.63
1:K:1073:HIS:NE2	1:L:1074:GLU:OE1	2.32	0.63
4:J:1417:HOH:O	1:L:1073:HIS:ND1	2.30	0.63
1:D:1021:ILE:O	1:F:1028:SER:OG	2.17	0.63
1:B:1195:ASP:OD2	1:C:1196:TYR:OH	2.17	0.63
1:H:1194:ALA:O	4:H:1422:HOH:O	2.16	0.63
1:F:1183:THR:O	1:F:1187:ASN:ND2	2.32	0.63
1:E:1279:GLU:OE2	1:E:1283:ARG:NH2	2.32	0.62
1:K:1111:GLU:OE2	1:L:1116:GLN:NE2	2.31	0.62
1:A:1279:GLU:OE2	1:A:1283:ARG:NH2	2.31	0.62
1:B:1024:ARG:NH1	4:B:1347:HOH:O	2.31	0.62
1:E:1083:ASP:OD1	1:E:1084:VAL:N	2.33	0.62
1:J:1205:GLN:N	4:L:1465:HOH:O	2.31	0.62
1:H:1066:GLN:NE2	1:I:1067:ASP:OD1	2.33	0.62
1:C:1198:SER:OG	1:C:1200:THR:OG1	2.17	0.62
1:K:1142:ASP:OD2	4:K:1446:HOH:O	2.16	0.62
1:J:1242:GLY:O	1:J:1274:ARG:NH2	2.33	0.62
1:J:1217:TYR:CE2	1:L:1217:TYR:CE2	2.87	0.62
1:A:1200:THR:OG1	1:C:1195:ASP:OD2	2.17	0.62
1:K:1227:ALA:O	1:L:1285:HIS:NE2	2.32	0.62
1:G:1038:GLN:NE2	4:G:1453:HOH:O	2.33	0.62
1:I:1237:GLY:O	1:I:1276:LYS:NZ	2.32	0.62
1:J:1228:ARG:NH1	4:J:1420:HOH:O	2.31	0.62
1:J:1087:HIS:NE2	1:K:1088:GLU:OE2	2.33	0.62
1:G:1127:THR:OG1	1:I:1125:ARG:NH2	2.33	0.61
1:J:1223:LYS:NZ	1:J:1225:VAL:O	2.33	0.61
1:B:1041:ASP:OD1	1:B:1042:VAL:N	2.33	0.61
1:H:1272:ARG:NE	1:I:1245:ASP:O	2.33	0.61
1:B:1048:LYS:O	1:B:1052:ALA:N	2.34	0.61
1:C:1024:ARG:NH2	4:C:1316:HOH:O	2.33	0.61
1:J:1076:ARG:NH1	1:K:1074:GLU:OE2	2.33	0.61
1:B:1066:GLN:NE2	1:C:1066:GLN:OE1	2.34	0.61
1:L:1216:SER:OG	1:L:1217:TYR:N	2.34	0.61
1:F:1048:LYS:O	1:F:1052:ALA:N	2.33	0.61
1:B:1229:GLN:O	1:B:1289:ASP:N	2.34	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1233:THR:OG1	4:D:1409:HOH:O	2.15	0.61
1:G:1027:PHE:N	4:G:1455:HOH:O	2.33	0.61
1:A:1104:ARG:O	4:B:1343:HOH:O	2.16	0.61
1:C:1240:ASN:ND2	4:C:1327:HOH:O	2.32	0.61
1:L:1212:ASN:OD1	1:L:1213:VAL:N	2.33	0.61
1:H:1279:GLU:OE1	1:I:1274:ARG:NE	2.33	0.60
1:C:1254:ASP:OD1	1:C:1254:ASP:N	2.34	0.60
1:D:1199:LYS:NZ	4:D:1421:HOH:O	2.34	0.60
1:H:1230:THR:OG1	1:H:1231:GLY:N	2.34	0.60
1:C:1111:GLU:O	1:C:1115:LEU:N	2.34	0.60
1:K:1209:SER:OG	1:L:1203:THR:O	2.19	0.60
1:L:1037:ALA:O	1:L:1040:THR:OG1	2.20	0.60
1:L:1251:ALA:O	4:L:1402:HOH:O	2.16	0.60
1:H:1193:GLN:NE2	4:H:1446:HOH:O	2.34	0.60
1:E:1104:ARG:NH2	1:F:1106:THR:OG1	2.35	0.60
1:I:1005:SER:OG	4:I:1450:HOH:O	2.17	0.60
1:C:1083:ASP:OD1	1:C:1084:VAL:N	2.34	0.60
1:G:1272:ARG:NH1	1:H:1245:ASP:OD1	2.34	0.60
1:A:1007:ASN:ND2	4:A:1450:HOH:O	2.34	0.60
1:J:1160:ARG:O	1:J:1163:THR:OG1	2.19	0.60
1:C:1132:ASN:ND2	4:C:1319:HOH:O	2.35	0.59
1:I:1007:ASN:OD1	1:I:1008:ASN:N	2.34	0.59
1:I:1266:ASN:OD1	1:K:1238:THR:OG1	2.20	0.59
1:F:1274:ARG:NE	4:F:1304:HOH:O	2.35	0.59
1:G:1144:GLU:O	1:G:1148:THR:OG1	2.19	0.59
1:E:1268:LEU:N	4:E:1401:HOH:O	2.34	0.59
1:B:1146:ARG:NH1	1:C:1144:GLU:OE2	2.35	0.59
1:A:1220:GLY:N	4:B:1349:HOH:O	2.35	0.59
1:I:1279:GLU:OE1	4:I:1434:HOH:O	2.16	0.59
1:J:1007:ASN:ND2	1:J:1054:GLN:OE1	2.36	0.59
1:J:1195:ASP:O	4:K:1430:HOH:O	2.17	0.59
1:J:1066:GLN:NE2	1:K:1067:ASP:OD1	2.35	0.59
1:A:1247:ASP:OD1	1:C:1273:ARG:NH2	2.35	0.59
1:A:1253:SER:OG	1:A:1257:THR:OG1	2.21	0.59
1:D:1242:GLY:O	1:D:1274:ARG:NH2	2.36	0.59
1:C:1279:GLU:OE2	1:C:1283:ARG:NH2	2.36	0.59
1:L:1209:SER:N	4:L:1464:HOH:O	2.36	0.59
1:B:1198:SER:OG	1:B:1201:ALA:N	2.36	0.59
1:D:1136:LEU:O	1:D:1140:VAL:N	2.36	0.58
1:G:1081:ARG:NH2	4:G:1414:HOH:O	2.35	0.58
1:G:1060:GLN:NE2	4:G:1445:HOH:O	2.37	0.58
4:A:1424:HOH:O	1:C:1160:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1142:ASP:O	1:A:1145:SER:OG	2.20	0.58
1:D:1123:ASP:O	1:D:1127:THR:OG1	2.22	0.58
1:J:1125:ARG:NH2	1:K:1127:THR:OG1	2.36	0.58
1:J:1139:ASP:OD1	1:J:1140:VAL:N	2.37	0.58
1:K:1063:ASN:OD1	1:L:1063:ASN:ND2	2.37	0.58
1:L:1018:ASP:O	1:L:1020:SER:N	2.36	0.58
1:D:1015:THR:O	1:D:1016:ARG:NH1	2.37	0.58
1:A:1272:ARG:NH2	1:B:1245:ASP:O	2.37	0.58
1:A:1076:ARG:NH1	1:B:1074:GLU:OE1	2.37	0.57
1:A:1227:ALA:O	1:B:1285:HIS:NE2	2.37	0.57
1:D:1228:ARG:NH2	4:D:1403:HOH:O	2.37	0.57
1:J:1272:ARG:NH1	1:K:1267:ALA:O	2.37	0.57
1:I:1152:LYS:NZ	4:I:1416:HOH:O	2.37	0.57
1:J:1062:LYS:NZ	1:K:1067:ASP:OD2	2.36	0.57
1:A:1137:GLN:O	1:A:1141:ASP:N	2.37	0.57
1:J:1019:ALA:N	4:J:1445:HOH:O	2.37	0.57
1:H:1011:VAL:O	4:H:1412:HOH:O	2.17	0.57
1:I:1111:GLU:OE2	4:I:1431:HOH:O	2.17	0.57
1:K:1255:THR:O	1:K:1257:THR:OG1	2.23	0.57
1:I:1165:GLU:OE2	4:I:1437:HOH:O	2.17	0.57
1:H:1104:ARG:NH2	1:I:1106:THR:OG1	2.37	0.57
1:B:1235:ALA:O	1:B:1276:LYS:NZ	2.38	0.57
1:I:1054:GLN:OE1	4:I:1430:HOH:O	2.17	0.56
1:G:1001:MET:O	1:I:1062:LYS:NZ	2.39	0.56
1:I:1188:ASN:ND2	4:I:1460:HOH:O	2.38	0.56
1:F:1242:GLY:O	1:F:1274:ARG:NH1	2.38	0.56
1:F:1086:ASP:OD1	4:F:1319:HOH:O	2.18	0.56
1:C:1034:TYR:O	1:C:1038:GLN:N	2.38	0.56
1:H:1062:LYS:NZ	1:H:1065:GLU:OE2	2.38	0.56
1:K:1250:PHE:CE1	1:K:1264:ILE:CG1	2.88	0.56
1:F:1081:ARG:NH1	4:F:1337:HOH:O	2.39	0.56
1:J:1175:VAL:N	4:J:1464:HOH:O	2.38	0.56
1:A:1195:ASP:OD2	1:B:1196:TYR:OH	2.23	0.56
1:H:1187:ASN:ND2	4:H:1437:HOH:O	2.38	0.56
1:B:1104:ARG:NH1	1:C:1102:ASN:OD1	2.38	0.56
1:D:1062:LYS:O	1:D:1066:GLN:N	2.39	0.56
1:H:1187:ASN:OD1	1:H:1188:ASN:N	2.38	0.56
1:D:1253:SER:OG	4:D:1406:HOH:O	2.18	0.56
1:J:1041:ASP:O	1:J:1045:ILE:N	2.38	0.56
4:B:1336:HOH:O	1:C:1073:HIS:ND1	2.33	0.56
1:F:1125:ARG:O	1:F:1128:THR:OG1	2.24	0.56
1:B:1279:GLU:OE2	1:B:1283:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1212:ASN:OD1	1:A:1213:VAL:N	2.38	0.55
1:D:1160:ARG:NH2	1:E:1162:THR:OG1	2.39	0.55
1:E:1103:VAL:O	1:E:1107:THR:OG1	2.23	0.55
1:J:1186:GLU:OE1	1:L:1181:ARG:NH2	2.39	0.55
1:G:1270:THR:OG1	1:I:1272:ARG:NH2	2.39	0.55
1:L:1256:TYR:O	1:L:1257:THR:OG1	2.25	0.55
1:J:1217:TYR:CE2	1:L:1217:TYR:CZ	2.78	0.55
1:C:1224:VAL:CG1	1:C:1224:VAL:O	2.55	0.55
1:D:1244:PHE:O	1:F:1236:THR:OG1	2.23	0.55
1:G:1195:ASP:OD1	1:H:1199:LYS:N	2.40	0.55
1:B:1258:GLN:NE2	1:B:1260:GLU:OE1	2.40	0.55
1:L:1165:GLU:OE2	4:L:1413:HOH:O	2.18	0.55
1:A:1074:GLU:OE1	1:C:1073:HIS:NE2	2.40	0.55
1:D:1034:TYR:OH	4:D:1408:HOH:O	2.18	0.55
1:B:1209:SER:OG	1:C:1205:GLN:OE1	2.26	0.54
1:F:1022:LEU:O	1:F:1024:ARG:N	2.40	0.54
1:L:1123:ASP:O	1:L:1127:THR:OG1	2.26	0.54
1:L:1041:ASP:O	1:L:1045:ILE:N	2.40	0.54
1:F:1058:ASP:OD1	1:F:1059:ALA:N	2.41	0.54
1:J:1256:TYR:OH	1:K:1253:SER:O	2.25	0.54
4:A:1402:HOH:O	1:C:1235:ALA:N	2.40	0.54
1:K:1199:LYS:NZ	4:K:1411:HOH:O	2.41	0.54
1:F:1108:ALA:O	1:F:1112:ILE:N	2.41	0.54
1:D:1060:GLN:NE2	1:F:1058:ASP:OD1	2.41	0.54
1:E:1197:VAL:N	4:E:1404:HOH:O	2.40	0.54
1:A:1087:HIS:ND1	4:A:1441:HOH:O	2.33	0.54
1:G:1195:ASP:OD1	1:H:1200:THR:N	2.41	0.54
1:E:1081:ARG:O	1:E:1085:ASP:N	2.40	0.54
1:A:1066:GLN:OE1	1:B:1066:GLN:NE2	2.41	0.54
1:B:1195:ASP:OD1	1:B:1196:TYR:N	2.40	0.54
1:I:1029:LYS:NZ	4:I:1403:HOH:O	2.42	0.53
1:B:1087:HIS:O	1:B:1091:ILE:N	2.42	0.53
1:L:1196:TYR:CZ	1:L:1198:SER:CB	2.91	0.53
1:B:1114:SER:OG	4:B:1363:HOH:O	2.19	0.53
1:L:1161:VAL:O	1:L:1165:GLU:N	2.42	0.53
1:J:1174:ASN:O	1:J:1178:LEU:N	2.41	0.53
1:E:1238:THR:N	4:E:1424:HOH:O	2.42	0.53
1:F:1254:ASP:N	1:F:1254:ASP:OD1	2.41	0.53
1:D:1007:ASN:OD1	1:D:1054:GLN:NE2	2.41	0.52
1:I:1189:ILE:O	1:I:1193:GLN:N	2.42	0.52
1:A:1241:LYS:NZ	4:A:1451:HOH:O	2.41	0.52
1:D:1212:ASN:O	1:E:1207:LEU:N	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:1262:GLN:O	1:K:1266:ASN:N	2.43	0.52
1:D:1245:ASP:O	4:D:1458:HOH:O	2.19	0.52
1:F:1079:GLN:NE2	4:F:1364:HOH:O	2.41	0.52
1:D:1005:SER:OG	4:D:1452:HOH:O	2.19	0.52
1:G:1240:ASN:O	1:G:1274:ARG:NH1	2.42	0.52
1:A:1170:SER:O	1:A:1173:THR:OG1	2.27	0.52
1:L:1240:ASN:N	4:L:1428:HOH:O	2.42	0.52
1:F:1063:ASN:OD1	1:F:1066:GLN:NE2	2.43	0.51
1:C:1114:SER:OG	4:C:1321:HOH:O	2.19	0.51
1:E:1275:THR:OG1	1:F:1271:GLU:OE2	2.27	0.51
1:C:1212:ASN:ND2	4:C:1344:HOH:O	2.43	0.51
1:H:1142:ASP:OD2	1:H:1143:HIS:ND1	2.43	0.51
1:E:1094:ASN:ND2	1:F:1095:THR:OG1	2.43	0.51
1:J:1279:GLU:OE1	1:K:1274:ARG:NE	2.42	0.51
1:K:1076:ARG:NH1	1:L:1074:GLU:OE2	2.43	0.51
1:J:1083:ASP:OD1	1:J:1084:VAL:N	2.44	0.51
1:H:1208:ALA:O	4:H:1402:HOH:O	2.19	0.51
1:C:1164:ALA:O	4:C:1323:HOH:O	2.19	0.51
1:H:1037:ALA:O	1:H:1040:THR:OG1	2.28	0.51
1:C:1242:GLY:O	1:C:1274:ARG:NH2	2.44	0.51
1:G:1254:ASP:OD1	1:G:1255:THR:N	2.44	0.51
1:B:1204:SER:O	4:B:1355:HOH:O	2.20	0.51
1:H:1101:LEU:O	1:H:1105:VAL:N	2.44	0.50
1:G:1173:THR:OG1	4:G:1419:HOH:O	2.19	0.50
1:H:1212:ASN:OD1	1:H:1213:VAL:N	2.45	0.50
1:G:1087:HIS:CD2	4:H:1454:HOH:O	2.64	0.50
1:F:1105:VAL:N	4:F:1367:HOH:O	2.44	0.50
1:I:1212:ASN:OD1	1:I:1213:VAL:N	2.44	0.50
1:A:1104:ARG:O	1:A:1107:THR:OG1	2.30	0.50
1:F:1186:GLU:OE1	4:F:1307:HOH:O	2.19	0.50
1:G:1204:SER:OG	4:G:1422:HOH:O	2.19	0.50
1:A:1024:ARG:O	4:A:1420:HOH:O	2.19	0.50
1:D:1199:LYS:NZ	4:F:1313:HOH:O	2.45	0.50
1:H:1273:ARG:O	1:H:1276:LYS:N	2.44	0.50
1:E:1224:VAL:O	1:F:1286:GLY:N	2.45	0.50
1:G:1022:LEU:O	4:G:1456:HOH:O	2.19	0.50
1:A:1022:LEU:O	4:A:1469:HOH:O	2.19	0.50
1:E:1238:THR:OG1	4:E:1424:HOH:O	2.19	0.50
1:I:1139:ASP:O	1:I:1143:HIS:N	2.45	0.50
1:G:1095:THR:O	1:G:1099:THR:OG1	2.30	0.50
1:E:1253:SER:OG	1:E:1254:ASP:OD1	2.30	0.50
1:H:1018:ASP:OD1	1:H:1018:ASP:N	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:1156:ALA:O	4:F:1302:HOH:O	2.19	0.50
1:E:1276:LYS:O	1:E:1280:ASP:N	2.45	0.49
1:C:1022:LEU:O	1:C:1024:ARG:N	2.45	0.49
1:I:1176:SER:OG	4:I:1421:HOH:O	2.20	0.49
1:L:1289:ASP:OD1	1:L:1289:ASP:N	2.44	0.49
1:J:1154:ILE:O	1:J:1158:ASN:ND2	2.45	0.49
1:K:1274:ARG:O	1:K:1278:LEU:N	2.46	0.49
1:E:1089:SER:OG	1:E:1090:ARG:N	2.45	0.49
1:J:1197:VAL:C	1:L:1197:VAL:CG2	2.78	0.49
1:G:1203:THR:OG1	4:G:1401:HOH:O	2.20	0.49
1:H:1123:ASP:O	1:H:1127:THR:OG1	2.30	0.49
1:H:1094:ASN:OD1	1:I:1095:THR:OG1	2.30	0.49
1:A:1067:ASP:OD2	1:C:1062:LYS:NZ	2.45	0.49
1:G:1151:THR:OG1	1:I:1150:ASN:ND2	2.46	0.49
1:D:1037:ALA:O	1:D:1040:THR:OG1	2.30	0.49
1:D:1272:ARG:NH2	1:E:1245:ASP:O	2.45	0.49
1:H:1150:ASN:ND2	3:I:1301:CL:CL	2.83	0.49
1:I:1128:THR:O	1:I:1132:ASN:N	2.45	0.49
1:J:1254:ASP:OD2	1:J:1254:ASP:N	2.46	0.49
1:E:1102:ASN:O	1:E:1106:THR:N	2.46	0.49
1:D:1216:SER:OG	1:D:1217:TYR:N	2.45	0.49
1:D:1078:LYS:NZ	4:D:1422:HOH:O	2.46	0.49
1:A:1153:ALA:O	1:A:1157:LEU:N	2.45	0.49
1:F:1104:ARG:O	1:F:1107:THR:OG1	2.31	0.49
1:A:1131:ASN:O	1:A:1134:SER:OG	2.31	0.49
1:A:1183:THR:OG1	1:C:1181:ARG:NH2	2.46	0.48
1:I:1048:LYS:O	1:I:1052:ALA:N	2.46	0.48
1:L:1198:SER:O	1:L:1205:GLN:NE2	2.46	0.48
1:J:1041:ASP:OD1	1:J:1042:VAL:N	2.46	0.48
1:J:1012:ILE:O	1:J:1013:GLN:NE2	2.45	0.48
1:D:1109:GLU:OE1	4:D:1428:HOH:O	2.20	0.48
1:F:1025:ASN:N	1:F:1025:ASN:OD1	2.46	0.48
1:I:1184:THR:O	1:I:1188:ASN:N	2.46	0.48
1:G:1074:GLU:OE1	1:I:1073:HIS:NE2	2.46	0.48
1:J:1028:SER:OG	1:K:1021:ILE:O	2.31	0.48
1:C:1252:VAL:N	1:C:1260:GLU:OE2	2.47	0.48
1:I:1196:TYR:O	4:I:1412:HOH:O	2.20	0.48
1:D:1060:GLN:NE2	1:F:1055:GLY:O	2.47	0.48
1:J:1157:LEU:O	1:J:1161:VAL:N	2.47	0.48
1:J:1170:SER:O	1:J:1173:THR:OG1	2.31	0.48
1:G:1055:GLY:O	1:H:1060:GLN:NE2	2.47	0.48
1:J:1150:ASN:OD1	4:J:1425:HOH:O	2.20	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:1041:ASP:O	1:L:1044:ALA:N	2.47	0.48
1:K:1237:GLY:O	1:K:1276:LYS:NZ	2.47	0.48
1:J:1037:ALA:O	1:J:1040:THR:OG1	2.32	0.48
1:G:1279:GLU:OE2	1:G:1283:ARG:NH2	2.47	0.48
1:G:1227:ALA:O	1:H:1285:HIS:NE2	2.47	0.48
1:D:1081:ARG:NH1	1:D:1085:ASP:OD1	2.46	0.48
1:E:1259:SER:N	4:E:1448:HOH:O	2.46	0.48
1:D:1010:VAL:N	1:D:1050:ASN:OD1	2.47	0.48
1:A:1181:ARG:O	1:A:1185:ALA:N	2.47	0.48
1:A:1247:ASP:N	4:A:1455:HOH:O	2.46	0.47
1:L:1174:ASN:O	1:L:1178:LEU:N	2.46	0.47
1:C:1036:ILE:O	4:C:1305:HOH:O	2.20	0.47
1:E:1108:ALA:O	1:E:1112:ILE:N	2.47	0.47
1:A:1231:GLY:N	4:A:1408:HOH:O	2.46	0.47
1:J:1144:GLU:OE1	1:L:1143:HIS:NE2	2.48	0.47
1:G:1224:VAL:O	1:H:1286:GLY:N	2.46	0.47
1:E:1254:ASP:N	1:E:1254:ASP:OD1	2.47	0.47
1:B:1063:ASN:OD1	1:B:1066:GLN:NE2	2.48	0.47
1:I:1258:GLN:NE2	1:J:1230:THR:O	2.48	0.47
1:K:1214:THR:CG2	1:K:1215:THR:OG1	2.63	0.47
1:E:1034:TYR:O	1:E:1038:GLN:N	2.47	0.47
1:H:1101:LEU:N	4:H:1432:HOH:O	2.47	0.47
1:G:1205:GLN:O	1:I:1212:ASN:N	2.48	0.46
1:F:1197:VAL:O	1:F:1199:LYS:NZ	2.48	0.46
1:H:1253:SER:OG	1:H:1257:THR:OG1	2.32	0.46
1:F:1018:ASP:OD1	1:F:1018:ASP:N	2.48	0.46
1:J:1231:GLY:O	1:K:1241:LYS:NZ	2.48	0.46
1:D:1247:ASP:N	4:D:1458:HOH:O	2.48	0.46
1:J:1123:ASP:O	1:J:1127:THR:OG1	2.33	0.46
1:G:1096:LYS:NZ	4:G:1442:HOH:O	2.47	0.46
1:C:1168:ILE:N	4:C:1323:HOH:O	2.48	0.46
1:E:1253:SER:OG	1:E:1254:ASP:N	2.49	0.46
1:A:1054:GLN:O	1:A:1058:ASP:N	2.49	0.46
1:C:1228:ARG:NH2	4:C:1308:HOH:O	2.49	0.46
1:H:1096:LYS:O	1:H:1099:THR:OG1	2.34	0.46
1:I:1221:GLY:N	4:I:1447:HOH:O	2.49	0.46
1:B:1048:LYS:NZ	1:C:1050:ASN:OD1	2.48	0.46
1:K:1090:ARG:NH2	4:K:1438:HOH:O	2.48	0.46
1:F:1104:ARG:NH2	4:F:1346:HOH:O	2.49	0.46
1:G:1102:ASN:O	1:G:1106:THR:N	2.49	0.45
1:E:1262:GLN:O	1:E:1266:ASN:N	2.49	0.45
1:H:1218:SER:N	1:I:1217:TYR:OH	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:1167:GLU:OE2	4:I:1424:HOH:O	2.21	0.45
1:E:1269:ILE:O	1:E:1273:ARG:N	2.49	0.45
1:D:1262:GLN:O	1:D:1266:ASN:N	2.50	0.45
1:E:1148:THR:O	1:E:1151:THR:OG1	2.35	0.45
1:J:1266:ASN:N	4:J:1456:HOH:O	2.50	0.45
1:G:1034:TYR:O	1:G:1037:ALA:N	2.50	0.45
1:J:1020:SER:OG	1:J:1022:LEU:N	2.50	0.45
1:A:1094:ASN:ND2	3:A:1303:CL:CL	2.87	0.45
1:A:1270:THR:OG1	1:C:1272:ARG:NH2	2.49	0.45
1:K:1170:SER:O	1:K:1173:THR:OG1	2.34	0.45
1:J:1176:SER:N	4:J:1464:HOH:O	2.48	0.45
1:A:1128:THR:OG1	4:A:1438:HOH:O	2.21	0.45
1:B:1055:GLY:O	1:B:1059:ALA:N	2.50	0.45
1:B:1168:ILE:O	1:B:1172:GLN:N	2.50	0.45
1:K:1262:GLN:N	1:K:1262:GLN:OE1	2.50	0.45
1:K:1025:ASN:ND2	1:K:1025:ASN:O	2.50	0.45
1:K:1087:HIS:O	1:K:1091:ILE:N	2.50	0.45
1:A:1182:VAL:N	4:A:1445:HOH:O	2.49	0.45
1:I:1158:ASN:O	1:I:1162:THR:OG1	2.35	0.45
1:G:1144:GLU:N	4:G:1408:HOH:O	2.50	0.44
1:B:1040:THR:O	4:B:1365:HOH:O	2.21	0.44
1:I:1034:TYR:OH	1:I:1038:GLN:OE1	2.35	0.44
1:H:1072:ASP:O	1:H:1076:ARG:NH1	2.51	0.44
1:A:1088:GLU:OE1	1:C:1087:HIS:NE2	2.50	0.44
1:D:1198:SER:O	4:D:1440:HOH:O	2.21	0.44
1:D:1195:ASP:OD2	1:E:1198:SER:OG	2.35	0.44
1:D:1105:VAL:O	1:D:1109:GLU:N	2.51	0.44
1:C:1212:ASN:OD1	1:C:1213:VAL:N	2.51	0.44
1:K:1214:THR:C	1:K:1215:THR:OG1	2.56	0.44
1:F:1074:GLU:OE2	4:F:1340:HOH:O	2.21	0.44
1:F:1074:GLU:O	1:F:1078:LYS:N	2.50	0.44
1:H:1129:ALA:O	1:H:1132:ASN:N	2.51	0.44
1:E:1007:ASN:N	1:E:1007:ASN:OD1	2.49	0.44
1:B:1161:VAL:O	1:B:1165:GLU:N	2.50	0.44
1:C:1011:VAL:O	1:C:1013:GLN:NE2	2.50	0.44
1:D:1025:ASN:N	4:D:1410:HOH:O	2.51	0.44
1:E:1050:ASN:OD1	1:E:1051:GLU:N	2.51	0.44
1:A:1256:TYR:OH	1:B:1253:SER:O	2.36	0.43
1:F:1111:GLU:O	4:F:1324:HOH:O	2.20	0.43
1:D:1094:ASN:OD1	1:E:1095:THR:OG1	2.37	0.43
1:J:1112:ILE:O	1:J:1116:GLN:N	2.51	0.43
1:A:1165:GLU:OE1	4:A:1424:HOH:O	2.21	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:1003:ASP:OD2	1:K:1005:SER:OG	2.36	0.43
1:I:1131:ASN:OD1	4:I:1461:HOH:O	2.21	0.43
1:K:1118:ASN:N	4:K:1439:HOH:O	2.51	0.43
1:G:1028:SER:N	4:H:1440:HOH:O	2.50	0.43
1:J:1048:LYS:O	1:J:1052:ALA:N	2.52	0.43
1:D:1160:ARG:O	1:D:1163:THR:OG1	2.36	0.43
1:B:1272:ARG:NH1	1:C:1245:ASP:O	2.51	0.43
1:K:1197:VAL:N	4:L:1461:HOH:O	2.51	0.43
1:H:1074:GLU:N	4:H:1431:HOH:O	2.51	0.43
1:F:1164:ALA:O	1:F:1168:ILE:N	2.51	0.43
1:A:1040:THR:OG1	1:A:1041:ASP:N	2.52	0.43
1:K:1109:GLU:O	4:K:1425:HOH:O	2.21	0.43
1:G:1125:ARG:NH1	4:G:1426:HOH:O	2.52	0.43
1:I:1285:HIS:CD2	1:I:1285:HIS:N	2.87	0.42
1:I:1280:ASP:OD1	4:I:1429:HOH:O	2.21	0.42
1:G:1197:VAL:N	4:G:1404:HOH:O	2.52	0.42
1:J:1144:GLU:OE2	1:L:1146:ARG:NH1	2.52	0.42
1:J:1117:THR:O	1:J:1120:SER:OG	2.37	0.42
1:A:1143:HIS:ND1	4:C:1336:HOH:O	2.37	0.42
1:B:1059:ALA:O	1:B:1063:ASN:ND2	2.53	0.42
1:C:1224:VAL:O	1:C:1225:VAL:CG2	2.68	0.42
1:F:1177:ALA:O	4:F:1301:HOH:O	2.22	0.42
1:A:1254:ASP:OD1	1:A:1255:THR:OG1	2.37	0.42
1:I:1254:ASP:N	1:I:1254:ASP:OD1	2.52	0.42
1:B:1099:THR:OG1	4:B:1312:HOH:O	2.21	0.42
1:L:1217:TYR:CD1	1:L:1218:SER:N	2.87	0.42
1:K:1214:THR:CG2	1:K:1214:THR:O	2.67	0.42
1:C:1223:LYS:N	4:C:1353:HOH:O	2.52	0.42
1:C:1263:ALA:O	1:C:1267:ALA:N	2.53	0.42
1:A:1037:ALA:O	1:A:1040:THR:OG1	2.38	0.42
1:K:1034:TYR:O	1:K:1038:GLN:N	2.53	0.42
1:A:1218:SER:O	1:B:1217:TYR:OH	2.38	0.42
1:K:1066:GLN:OE1	1:L:1066:GLN:NE2	2.52	0.41
1:I:1027:PHE:O	4:I:1446:HOH:O	2.22	0.41
1:L:1182:VAL:O	1:L:1186:GLU:N	2.53	0.41
1:H:1142:ASP:O	1:H:1145:SER:OG	2.38	0.41
1:J:1180:GLY:O	1:J:1184:THR:OG1	2.39	0.41
1:L:1183:THR:OG1	4:L:1431:HOH:O	2.22	0.41
1:G:1183:THR:OG1	1:I:1181:ARG:NH2	2.53	0.41
1:A:1112:ILE:O	1:A:1116:GLN:N	2.53	0.41
1:K:1244:PHE:O	4:K:1450:HOH:O	2.21	0.41
1:K:1274:ARG:O	1:K:1277:ALA:N	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1014:ALA:N	1:C:1041:ASP:OD2	2.54	0.41
1:H:1281:ALA:O	4:H:1419:HOH:O	2.22	0.41
1:J:1127:THR:O	1:J:1131:ASN:ND2	2.54	0.41
1:D:1237:GLY:CA	4:D:1431:HOH:O	2.68	0.41
1:I:1072:ASP:O	1:I:1076:ARG:N	2.54	0.41
1:I:1206:SER:OG	1:I:1207:LEU:N	2.54	0.41
1:C:1274:ARG:O	1:C:1278:LEU:N	2.54	0.41
1:H:1066:GLN:NE2	1:I:1063:ASN:O	2.54	0.41
1:H:1211:LEU:O	1:H:1217:TYR:OH	2.39	0.41
1:J:1274:ARG:O	1:J:1277:ALA:N	2.54	0.40
1:D:1223:LYS:NZ	1:E:1285:HIS:O	2.54	0.40
1:C:1236:THR:OG1	1:C:1237:GLY:N	2.54	0.40
1:C:1101:LEU:O	1:C:1104:ARG:N	2.54	0.40
1:D:1260:GLU:OE1	4:D:1461:HOH:O	2.22	0.40
1:J:1212:ASN:OD1	1:J:1213:VAL:N	2.54	0.40
1:K:1046:ALA:O	1:K:1050:ASN:ND2	2.55	0.40
1:H:1010:VAL:N	1:H:1050:ASN:OD1	2.54	0.40
1:F:1047:GLY:O	1:F:1051:GLU:N	2.54	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:1244:PHE:O	4:F:1345:HOH:O[1_455]	1.98	0.22
1:J:1244:PHE:N	4:F:1345:HOH:O[1_455]	2.04	0.16
4:B:1346:HOH:O	4:D:1419:HOH:O[1_446]	2.06	0.14
1:F:1234:ALA:O	4:L:1408:HOH:O[1_655]	2.16	0.04
4:B:1338:HOH:O	4:D:1465:HOH:O[1_446]	2.18	0.02
1:A:1146:ARG:NH2	1:I:1025:ASN:OD1[1_474]	2.19	0.01
1:E:1024:ARG:NE	1:K:1142:ASP:OD1[1_636]	2.19	0.01

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	287/300 (96%)	276 (96%)	11 (4%)	0	100	100
1	B	287/300 (96%)	279 (97%)	8 (3%)	0	100	100
1	C	287/300 (96%)	276 (96%)	11 (4%)	0	100	100
1	D	287/300 (96%)	281 (98%)	6 (2%)	0	100	100
1	E	287/300 (96%)	277 (96%)	10 (4%)	0	100	100
1	F	287/300 (96%)	274 (96%)	13 (4%)	0	100	100
1	G	287/300 (96%)	281 (98%)	6 (2%)	0	100	100
1	H	287/300 (96%)	278 (97%)	9 (3%)	0	100	100
1	I	287/300 (96%)	277 (96%)	10 (4%)	0	100	100
1	J	287/300 (96%)	275 (96%)	12 (4%)	0	100	100
1	K	287/300 (96%)	273 (95%)	14 (5%)	0	100	100
1	L	287/300 (96%)	270 (94%)	16 (6%)	1 (0%)	50	82
All	All	3444/3600 (96%)	3317 (96%)	126 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1019	ALA

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	229/238 (96%)	193 (84%)	36 (16%)	4	10
1	B	229/238 (96%)	191 (83%)	38 (17%)	3	8
1	C	229/238 (96%)	189 (82%)	40 (18%)	3	7
1	D	229/238 (96%)	196 (86%)	33 (14%)	5	12
1	E	229/238 (96%)	194 (85%)	35 (15%)	4	10
1	F	229/238 (96%)	198 (86%)	31 (14%)	6	13
1	G	229/238 (96%)	193 (84%)	36 (16%)	4	10
1	H	229/238 (96%)	183 (80%)	46 (20%)	2	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	229/238 (96%)	194 (85%)	35 (15%)	4	10
1	J	229/238 (96%)	188 (82%)	41 (18%)	2	7
1	K	229/238 (96%)	182 (80%)	47 (20%)	2	5
1	L	229/238 (96%)	183 (80%)	46 (20%)	2	5
All	All	2748/2856 (96%)	2284 (83%)	464 (17%)	3	8

All (464) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1005	SER
1	A	1011	VAL
1	A	1015	THR
1	A	1016	ARG
1	A	1017	LEU
1	A	1018	ASP
1	A	1020	SER
1	A	1036	ILE
1	A	1073	HIS
1	A	1078	LYS
1	A	1082	ILE
1	A	1084	VAL
1	A	1085	ASP
1	A	1092	THR
1	A	1098	ILE
1	A	1099	THR
1	A	1111	GLU
1	A	1127	THR
1	A	1148	THR
1	A	1157	LEU
1	A	1175	VAL
1	A	1179	ASP
1	A	1189	ILE
1	A	1195	ASP
1	A	1196	TYR
1	A	1199	LYS
1	A	1200	THR
1	A	1203	THR
1	A	1213	VAL
1	A	1216	SER
1	A	1219	VAL
1	A	1249	THR

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Mol	Chain	Res	Type
1	A	1255	THR
1	A	1276	LYS
1	A	1280	ASP
1	A	1282	LEU
1	B	1010	VAL
1	B	1016	ARG
1	B	1017	LEU
1	B	1029	LYS
1	B	1032	LEU
1	B	1035	VAL
1	B	1054	GLN
1	B	1077	ILE
1	B	1078	LYS
1	B	1082	ILE
1	B	1085	ASP
1	B	1088	GLU
1	B	1092	THR
1	B	1096	LYS
1	B	1098	ILE
1	B	1117	THR
1	B	1119	VAL
1	B	1123	ASP
1	B	1127	THR
1	B	1151	THR
1	B	1154	ILE
1	B	1155	THR
1	B	1195	ASP
1	B	1196	TYR
1	B	1198	SER
1	B	1211	LEU
1	B	1215	THR
1	B	1219	VAL
1	B	1222	LYS
1	B	1228	ARG
1	B	1236	THR
1	B	1238	THR
1	B	1249	THR
1	B	1250	PHE
1	B	1256	TYR
1	B	1257	THR
1	B	1259	SER
1	B	1260	GLU

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Mol	Chain	Res	Type
1	C	1015	THR
1	C	1020	SER
1	C	1025	ASN
1	C	1035	VAL
1	C	1048	LYS
1	C	1051	GLU
1	C	1054	GLN
1	C	1068	VAL
1	C	1069	GLU
1	C	1081	ARG
1	C	1083	ASP
1	C	1095	THR
1	C	1106	THR
1	C	1114	SER
1	C	1115	LEU
1	C	1123	ASP
1	C	1133	ILE
1	C	1141	ASP
1	C	1148	THR
1	C	1157	LEU
1	C	1162	THR
1	C	1165	GLU
1	C	1171	LEU
1	C	1174	ASN
1	C	1176	SER
1	C	1179	ASP
1	C	1182	VAL
1	C	1192	LEU
1	C	1196	TYR
1	C	1197	VAL
1	C	1203	THR
1	C	1214	THR
1	C	1236	THR
1	C	1248	LEU
1	C	1249	THR
1	C	1250	PHE
1	C	1254	ASP
1	C	1255	THR
1	C	1275	THR
1	C	1276	LYS
1	D	1005	SER
1	D	1016	ARG

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Mol	Chain	Res	Type
1	D	1017	LEU
1	D	1024	ARG
1	D	1048	LYS
1	D	1051	GLU
1	D	1054	GLN
1	D	1070	LEU
1	D	1084	VAL
1	D	1141	ASP
1	D	1143	HIS
1	D	1145	SER
1	D	1155	THR
1	D	1158	ASN
1	D	1159	VAL
1	D	1160	ARG
1	D	1161	VAL
1	D	1171	LEU
1	D	1178	LEU
1	D	1183	THR
1	D	1196	TYR
1	D	1198	SER
1	D	1200	THR
1	D	1219	VAL
1	D	1224	VAL
1	D	1244	PHE
1	D	1248	LEU
1	D	1249	THR
1	D	1266	ASN
1	D	1274	ARG
1	D	1275	THR
1	D	1288	ILE
1	D	1289	ASP
1	E	1007	ASN
1	E	1015	THR
1	E	1024	ARG
1	E	1040	THR
1	E	1067	ASP
1	E	1080	LEU
1	E	1086	ASP
1	E	1119	VAL
1	E	1127	THR
1	E	1132	ASN
1	E	1140	VAL

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Mol	Chain	Res	Type
1	E	1155	THR
1	E	1159	VAL
1	E	1163	THR
1	E	1174	ASN
1	E	1178	LEU
1	E	1181	ARG
1	E	1183	THR
1	E	1186	GLU
1	E	1192	LEU
1	E	1195	ASP
1	E	1196	TYR
1	E	1211	LEU
1	E	1216	SER
1	E	1222	LYS
1	E	1228	ARG
1	E	1236	THR
1	E	1240	ASN
1	E	1248	LEU
1	E	1249	THR
1	E	1254	ASP
1	E	1257	THR
1	E	1258	GLN
1	E	1276	LYS
1	E	1289	ASP
1	F	1005	SER
1	F	1010	VAL
1	F	1018	ASP
1	F	1024	ARG
1	F	1025	ASN
1	F	1028	SER
1	F	1038	GLN
1	F	1058	ASP
1	F	1063	ASN
1	F	1069	GLU
1	F	1092	THR
1	F	1132	ASN
1	F	1141	ASP
1	F	1145	SER
1	F	1148	THR
1	F	1154	ILE
1	F	1170	SER
1	F	1178	LEU

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Mol	Chain	Res	Type
1	F	1196	TYR
1	F	1200	THR
1	F	1214	THR
1	F	1236	THR
1	F	1248	LEU
1	F	1250	PHE
1	F	1252	VAL
1	F	1254	ASP
1	F	1255	THR
1	F	1257	THR
1	F	1274	ARG
1	F	1276	LYS
1	F	1280	ASP
1	G	1012	ILE
1	G	1015	THR
1	G	1017	LEU
1	G	1021	ILE
1	G	1022	LEU
1	G	1025	ASN
1	G	1030	SER
1	G	1036	ILE
1	G	1058	ASP
1	G	1068	VAL
1	G	1080	LEU
1	G	1095	THR
1	G	1107	THR
1	G	1127	THR
1	G	1128	THR
1	G	1133	ILE
1	G	1144	GLU
1	G	1148	THR
1	G	1157	LEU
1	G	1181	ARG
1	G	1183	THR
1	G	1196	TYR
1	G	1197	VAL
1	G	1214	THR
1	G	1243	VAL
1	G	1248	LEU
1	G	1250	PHE
1	G	1252	VAL
1	G	1255	THR

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Mol	Chain	Res	Type
1	G	1257	THR
1	G	1260	GLU
1	G	1274	ARG
1	G	1276	LYS
1	G	1278	LEU
1	G	1280	ASP
1	G	1288	ILE
1	H	1003	ASP
1	H	1010	VAL
1	H	1011	VAL
1	H	1015	THR
1	H	1016	ARG
1	H	1017	LEU
1	H	1018	ASP
1	H	1021	ILE
1	H	1025	ASN
1	H	1041	ASP
1	H	1064	ASP
1	H	1068	VAL
1	H	1072	ASP
1	H	1074	GLU
1	H	1082	ILE
1	H	1083	ASP
1	H	1084	VAL
1	H	1095	THR
1	H	1096	LYS
1	H	1103	VAL
1	H	1112	ILE
1	H	1128	THR
1	H	1167	GLU
1	H	1188	ASN
1	H	1189	ILE
1	H	1196	TYR
1	H	1197	VAL
1	H	1198	SER
1	H	1204	SER
1	H	1209	SER
1	H	1213	VAL
1	H	1214	THR
1	H	1215	THR
1	H	1219	VAL
1	H	1224	VAL

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Mol	Chain	Res	Type
1	H	1238	THR
1	H	1248	LEU
1	H	1252	VAL
1	H	1254	ASP
1	H	1255	THR
1	H	1257	THR
1	H	1264	ILE
1	H	1273	ARG
1	H	1283	ARG
1	H	1288	ILE
1	H	1289	ASP
1	I	1001	MET
1	I	1011	VAL
1	I	1012	ILE
1	I	1016	ARG
1	I	1020	SER
1	I	1028	SER
1	I	1030	SER
1	I	1038	GLN
1	I	1045	ILE
1	I	1067	ASP
1	I	1081	ARG
1	I	1088	GLU
1	I	1089	SER
1	I	1109	GLU
1	I	1119	VAL
1	I	1122	LEU
1	I	1123	ASP
1	I	1139	ASP
1	I	1140	VAL
1	I	1143	HIS
1	I	1173	THR
1	I	1184	THR
1	I	1219	VAL
1	I	1228	ARG
1	I	1229	GLN
1	I	1230	THR
1	I	1233	THR
1	I	1238	THR
1	I	1249	THR
1	I	1256	TYR
1	I	1257	THR

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Mol	Chain	Res	Type
1	I	1266	ASN
1	I	1270	THR
1	I	1287	LEU
1	I	1289	ASP
1	J	1006	LEU
1	J	1007	ASN
1	J	1010	VAL
1	J	1012	ILE
1	J	1013	GLN
1	J	1015	THR
1	J	1020	SER
1	J	1022	LEU
1	J	1028	SER
1	J	1032	LEU
1	J	1035	VAL
1	J	1054	GLN
1	J	1068	VAL
1	J	1084	VAL
1	J	1088	GLU
1	J	1092	THR
1	J	1095	THR
1	J	1099	THR
1	J	1112	ILE
1	J	1114	SER
1	J	1123	ASP
1	J	1141	ASP
1	J	1143	HIS
1	J	1157	LEU
1	J	1159	VAL
1	J	1182	VAL
1	J	1184	THR
1	J	1192	LEU
1	J	1197	VAL
1	J	1213	VAL
1	J	1241	LYS
1	J	1250	PHE
1	J	1254	ASP
1	J	1255	THR
1	J	1257	THR
1	J	1259	SER
1	J	1261	ILE
1	J	1270	THR

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Mol	Chain	Res	Type
1	J	1278	LEU
1	J	1282	LEU
1	J	1283	ARG
1	K	1017	LEU
1	K	1021	ILE
1	K	1024	ARG
1	K	1025	ASN
1	K	1026	VAL
1	K	1032	LEU
1	K	1033	LEU
1	K	1038	GLN
1	K	1062	LYS
1	K	1077	ILE
1	K	1082	ILE
1	K	1102	ASN
1	K	1103	VAL
1	K	1105	VAL
1	K	1106	THR
1	K	1114	SER
1	K	1115	LEU
1	K	1117	THR
1	K	1133	ILE
1	K	1136	LEU
1	K	1145	SER
1	K	1147	ILE
1	K	1155	THR
1	K	1159	VAL
1	K	1162	THR
1	K	1165	GLU
1	K	1192	LEU
1	K	1195	ASP
1	K	1196	TYR
1	K	1197	VAL
1	K	1200	THR
1	K	1203	THR
1	K	1212	ASN
1	K	1215	THR
1	K	1217	TYR
1	K	1219	VAL
1	K	1228	ARG
1	K	1230	THR
1	K	1243	VAL

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Mol	Chain	Res	Type
1	K	1244	PHE
1	K	1245	ASP
1	K	1252	VAL
1	K	1253	SER
1	K	1256	TYR
1	K	1258	GLN
1	K	1260	GLU
1	K	1274	ARG
1	L	1001	MET
1	L	1017	LEU
1	L	1022	LEU
1	L	1027	PHE
1	L	1028	SER
1	L	1029	LYS
1	L	1035	VAL
1	L	1036	ILE
1	L	1048	LYS
1	L	1067	ASP
1	L	1070	LEU
1	L	1078	LYS
1	L	1079	GLN
1	L	1080	LEU
1	L	1109	GLU
1	L	1117	THR
1	L	1119	VAL
1	L	1122	LEU
1	L	1127	THR
1	L	1142	ASP
1	L	1144	GLU
1	L	1145	SER
1	L	1158	ASN
1	L	1162	THR
1	L	1176	SER
1	L	1179	ASP
1	L	1195	ASP
1	L	1197	VAL
1	L	1198	SER
1	L	1204	SER
1	L	1213	VAL
1	L	1214	THR
1	L	1216	SER
1	L	1228	ARG

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Mol	Chain	Res	Type
1	L	1229	GLN
1	L	1238	THR
1	L	1240	ASN
1	L	1243	VAL
1	L	1249	THR
1	L	1250	PHE
1	L	1253	SER
1	L	1256	TYR
1	L	1271	GLU
1	L	1273	ARG
1	L	1278	LEU
1	L	1289	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 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.

5.7 Other polymers ⓘ

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	289/300 (96%)	0.15	5 (1%) 67 73	29, 61, 89, 114	0
1	B	289/300 (96%)	0.22	8 (2%) 50 56	29, 59, 80, 96	0
1	C	289/300 (96%)	0.19	9 (3%) 47 52	26, 64, 92, 122	0
1	D	289/300 (96%)	0.31	8 (2%) 50 56	26, 73, 101, 118	0
1	E	289/300 (96%)	0.28	6 (2%) 60 67	28, 64, 93, 115	0
1	F	289/300 (96%)	0.25	10 (3%) 42 47	28, 60, 98, 124	0
1	G	289/300 (96%)	0.30	8 (2%) 50 56	33, 67, 100, 141	0
1	H	289/300 (96%)	0.29	8 (2%) 50 56	32, 68, 99, 114	0
1	I	289/300 (96%)	0.43	6 (2%) 60 67	33, 65, 97, 125	0
1	J	289/300 (96%)	0.35	12 (4%) 35 39	36, 67, 97, 116	0
1	K	289/300 (96%)	0.27	12 (4%) 35 39	37, 66, 102, 123	0
1	L	289/300 (96%)	0.33	12 (4%) 35 39	39, 65, 99, 119	0
All	All	3468/3600 (96%)	0.28	104 (2%) 48 54	26, 65, 97, 141	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1257	THR	9.5
1	L	1257	THR	6.5
1	L	1248	LEU	6.0
1	G	1246	ALA	5.8
1	B	1249	THR	5.3
1	I	1246	ALA	5.3
1	J	1251	ALA	5.1
1	G	1024	ARG	5.1
1	A	1251	ALA	5.0
1	K	1019	ALA	4.9
1	G	1251	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	I	1258	GLN	4.8
1	B	1014	ALA	4.6
1	C	1019	ALA	4.2
1	J	1083	ASP	3.9
1	K	1243	VAL	3.8
1	J	1014	ALA	3.7
1	B	1248	LEU	3.6
1	J	1255	THR	3.5
1	K	1026	VAL	3.5
1	B	1011	VAL	3.5
1	H	1026	VAL	3.3
1	J	1231	GLY	3.2
1	L	1018	ASP	3.2
1	G	1231	GLY	3.1
1	I	1248	LEU	3.0
1	K	1064	ASP	3.0
1	L	1231	GLY	3.0
1	D	1002	ALA	3.0
1	G	1014	ALA	2.9
1	B	1015	THR	2.9
1	K	1250	PHE	2.9
1	F	1085	ASP	2.8
1	J	1135	ALA	2.8
1	H	1207	LEU	2.8
1	L	1253	SER	2.8
1	I	1011	VAL	2.8
1	L	1216	SER	2.7
1	L	1270	THR	2.7
1	F	1002	ALA	2.7
1	L	1249	THR	2.7
1	D	1058	ASP	2.6
1	F	1251	ALA	2.6
1	H	1235	ALA	2.6
1	G	1017	LEU	2.6
1	F	1139	ASP	2.6
1	E	1064	ASP	2.6
1	J	1217	TYR	2.6
1	E	1173	THR	2.6
1	K	1252	VAL	2.6
1	B	1246	ALA	2.5
1	C	1110	GLY	2.5
1	A	1003	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	1113	ALA	2.5
1	L	1254	ASP	2.5
1	L	1246	ALA	2.5
1	D	1064	ASP	2.4
1	J	1214	THR	2.4
1	C	1014	ALA	2.4
1	J	1289	ASP	2.4
1	C	1027	PHE	2.4
1	C	1251	ALA	2.4
1	E	1019	ALA	2.3
1	K	1222	LYS	2.3
1	L	1239	ALA	2.3
1	J	1230	THR	2.3
1	K	1011	VAL	2.3
1	B	1251	ALA	2.3
1	K	1251	ALA	2.3
1	C	1112	ILE	2.2
1	F	1020	SER	2.2
1	A	1018	ASP	2.2
1	C	1018	ASP	2.2
1	J	1229	GLN	2.2
1	K	1245	ASP	2.2
1	F	1014	ALA	2.2
1	K	1215	THR	2.2
1	D	1149	ALA	2.2
1	L	1259	SER	2.2
1	D	1245	ASP	2.2
1	C	1192	LEU	2.2
1	F	1034	TYR	2.2
1	H	1243	VAL	2.2
1	H	1246	ALA	2.2
1	G	1221	GLY	2.2
1	D	1246	ALA	2.1
1	F	1004	PRO	2.1
1	K	1247	ASP	2.1
1	D	1017	LEU	2.1
1	A	1061	VAL	2.1
1	J	1015	THR	2.1
1	D	1085	ASP	2.1
1	C	1020	SER	2.1
1	E	1010	VAL	2.1
1	B	1017	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	1245	ASP	2.0
1	H	1280	ASP	2.0
1	G	1269	ILE	2.0
1	H	1032	LEU	2.0
1	E	1248	LEU	2.0
1	E	1065	GLU	2.0
1	A	1108	ALA	2.0
1	F	1029	LYS	2.0
1	F	1030	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CL	I	1301	1/1	0.87	15.29	171,171,171,171	0
2	CA	J	1301	1/1	0.24	1.87	99,99,99,99	0
3	CL	A	1302	1/1	0.12	-0.74	50,50,50,50	0
2	CA	E	1301	1/1	0.15	-0.76	54,54,54,54	0
3	CL	A	1303	1/1	0.09	-2.02	60,60,60,60	0
2	CA	A	1301	1/1	0.09	-2.20	79,79,79,79	0
3	CL	L	1301	1/1	0.10	-2.23	49,49,49,49	0
3	CL	H	1301	1/1	0.08	-2.37	38,38,38,38	0
3	CL	E	1302	1/1	0.10	-2.41	61,61,61,61	0
3	CL	K	1301	1/1	0.06	-3.86	52,52,52,52	0
3	CL	D	1301	1/1	0.08	-3.96	58,58,58,58	0
2	CA	G	1301	1/1	0.05	-4.51	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.