



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:49 AM UTC

PDB ID : 4KI3 / pdb_00004ki3
Title : 1.70 Angstrom resolution crystal structure of outer-membrane lipoprotein carrier protein (lolA) from Yersinia pestis CO92
Authors : Halavaty, A.S.; Wawrzak, Z.; Kudritska, M.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2013-05-01
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

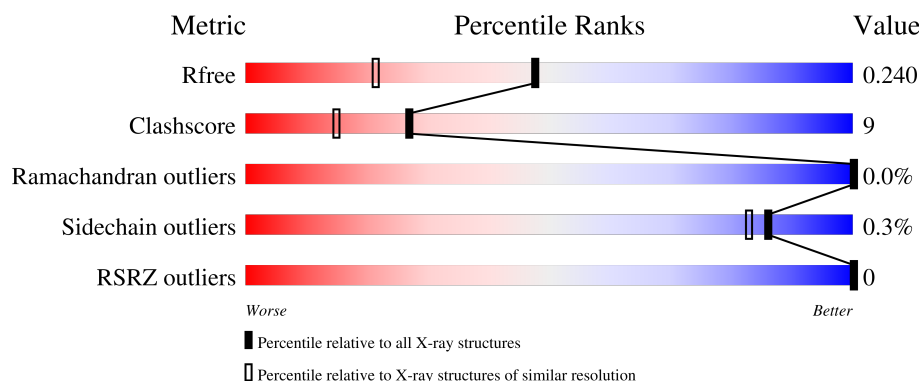
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	184	 79% 17% .
1	B	184	 73% 18% 8%
1	C	184	 79% 17% .
1	D	184	 84% 12% ..
1	E	184	 77% 15% 8%

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Mol	Chain	Length	Quality of chain
1	F	184	 83% 12% . .
1	G	184	 81% 16% . .
1	H	184	 77% 16% . 7%
1	I	184	 82% 16% .
1	J	184	 79% 16% . .
1	K	184	 76% 16% . 7%
1	L	184	 78% 17% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	H	301	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19260 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 Outer-membrane lipoprotein carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	12	0
			1490	933	251	304	2			
1	B	169	Total	C	N	O	S	0	14	0
			1453	913	248	289	3			
1	C	177	Total	C	N	O	S	0	12	0
			1491	936	253	299	3			
1	D	179	Total	C	N	O	S	0	14	0
			1524	950	260	312	2			
1	E	169	Total	C	N	O	S	0	9	0
			1409	887	237	283	2			
1	F	177	Total	C	N	O	S	0	11	0
			1482	928	250	301	3			
1	G	179	Total	C	N	O	S	0	15	0
			1520	950	253	315	2			
1	H	172	Total	C	N	O	S	0	10	0
			1434	901	241	290	2			
1	I	180	Total	C	N	O	S	0	10	0
			1494	937	252	302	3			
1	J	177	Total	C	N	O	S	0	13	0
			1503	944	252	304	3			
1	K	171	Total	C	N	O	S	0	5	0
			1389	874	232	280	3			
1	L	176	Total	C	N	O	S	0	10	0
			1464	915	248	298	3			

There are 24 discrepancies between the modelled and reference sequences:

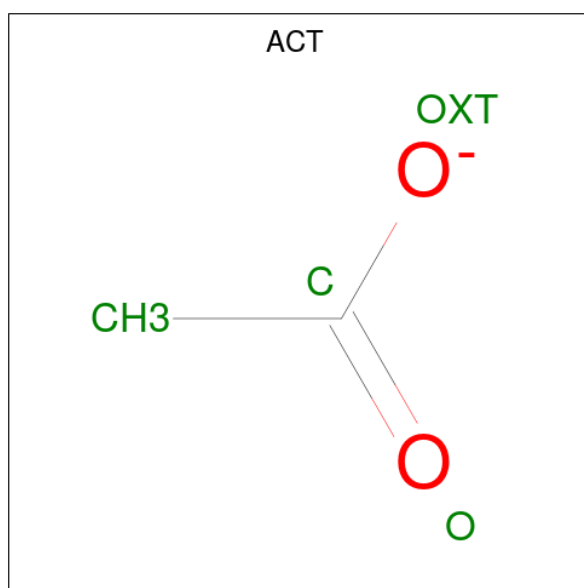
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	-	expression tag	UNP E8P443
A	20	ASN	-	expression tag	UNP E8P443
B	19	SER	-	expression tag	UNP E8P443
B	20	ASN	-	expression tag	UNP E8P443
C	19	SER	-	expression tag	UNP E8P443

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ASN	-	expression tag	UNP E8P443
D	19	SER	-	expression tag	UNP E8P443
D	20	ASN	-	expression tag	UNP E8P443
E	19	SER	-	expression tag	UNP E8P443
E	20	ASN	-	expression tag	UNP E8P443
F	19	SER	-	expression tag	UNP E8P443
F	20	ASN	-	expression tag	UNP E8P443
G	19	SER	-	expression tag	UNP E8P443
G	20	ASN	-	expression tag	UNP E8P443
H	19	SER	-	expression tag	UNP E8P443
H	20	ASN	-	expression tag	UNP E8P443
I	19	SER	-	expression tag	UNP E8P443
I	20	ASN	-	expression tag	UNP E8P443
J	19	SER	-	expression tag	UNP E8P443
J	20	ASN	-	expression tag	UNP E8P443
K	19	SER	-	expression tag	UNP E8P443
K	20	ASN	-	expression tag	UNP E8P443
L	19	SER	-	expression tag	UNP E8P443
L	20	ASN	-	expression tag	UNP E8P443

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



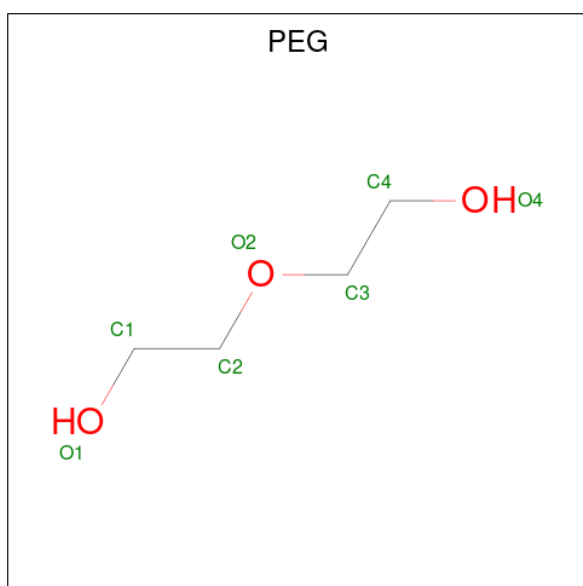
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	1
			14	8	6		
3	J	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	143	Total	O	0	3
			144	144		
5	B	137	Total	O	0	5
			141	141		
5	C	122	Total	O	0	7
			128	128		
5	D	146	Total	O	0	8
			153	153		
5	E	100	Total	O	0	2
			102	102		
5	F	116	Total	O	0	8
			119	119		
5	G	133	Total	O	0	8
			139	139		
5	H	146	Total	O	0	5
			149	149		
5	I	137	Total	O	0	3
			138	138		
5	J	104	Total	O	0	4
			108	108		

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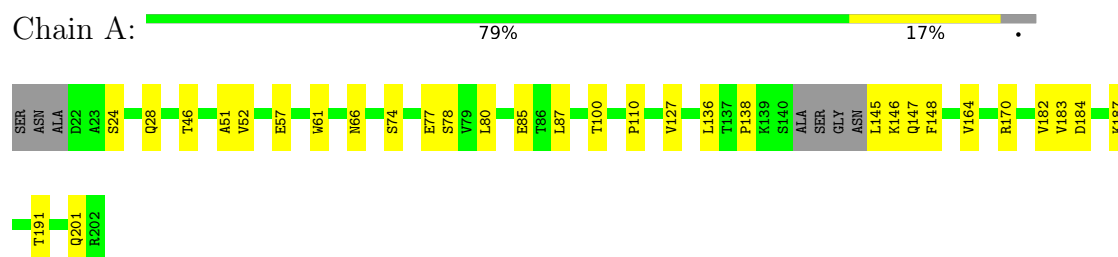
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	107	Total 109	O 109	0	3
5	L	106	Total 109	O 109	0	3

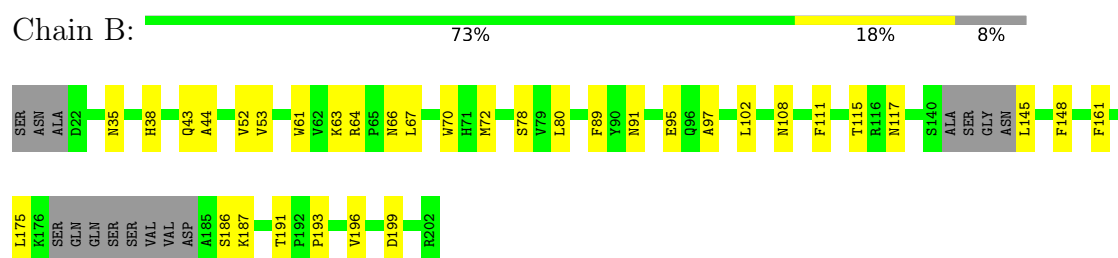
3 Residue-property plots

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.

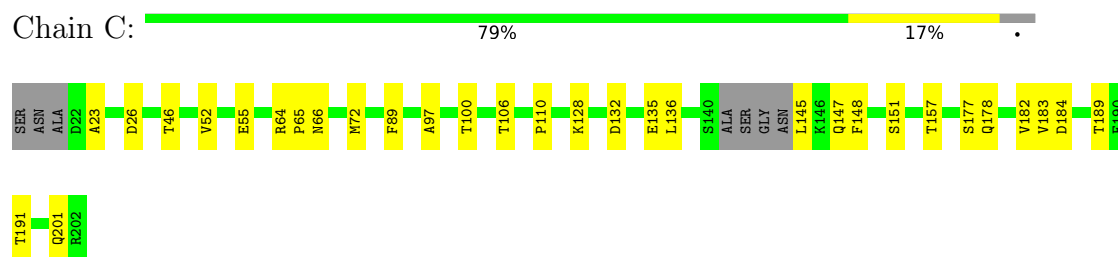
- Molecule 1: Outer-membrane lipoprotein carrier protein



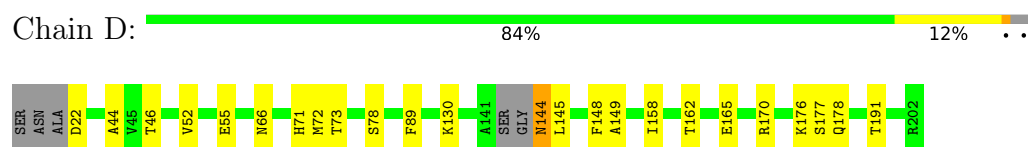
- Molecule 1: Outer-membrane lipoprotein carrier protein



- Molecule 1: Outer-membrane lipoprotein carrier protein

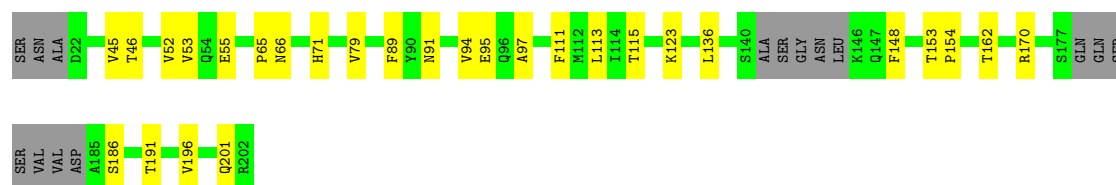


- Molecule 1: Outer-membrane lipoprotein carrier protein



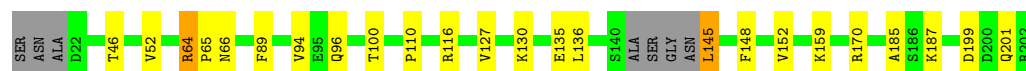
- Molecule 1: Outer-membrane lipoprotein carrier protein

Chain E: 



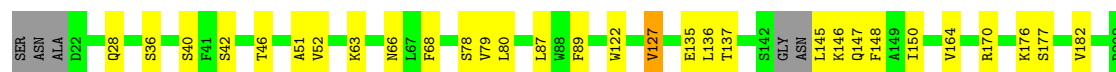
- Molecule 1: Outer-membrane lipoprotein carrier protein

Chain F: 



- Molecule 1: Outer-membrane lipoprotein carrier protein

Chain G: 



- Molecule 1: Outer-membrane lipoprotein carrier protein

Chain H: 



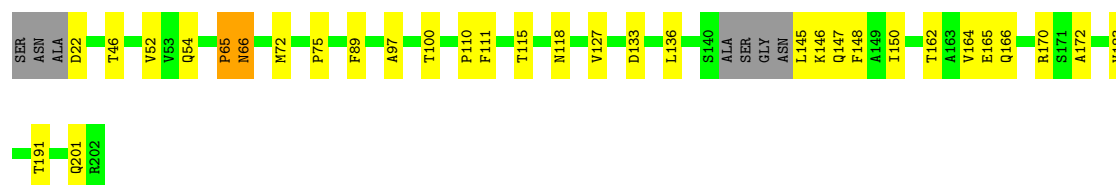
- Molecule 1: Outer-membrane lipoprotein carrier protein

Chain I: 

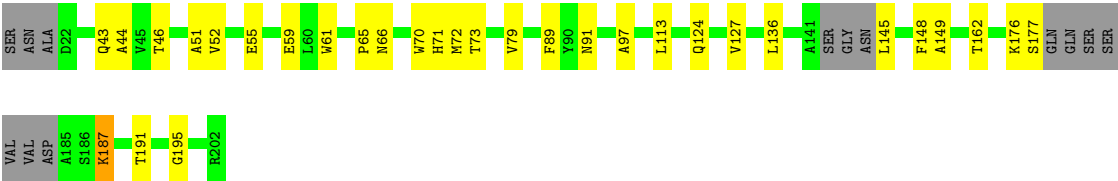


- Molecule 1: Outer-membrane lipoprotein carrier protein

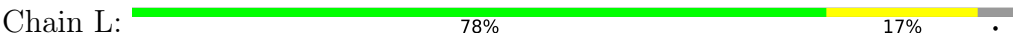
Chain J: 



● Molecule 1: Outer-membrane lipoprotein carrier protein



● Molecule 1: Outer-membrane lipoprotein carrier protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.20Å 67.13Å 132.56Å 94.30° 94.01° 120.01°	Depositor
Resolution (Å)	29.09 – 1.70 29.09 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.8 (29.09-1.70) 93.8 (29.09-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.204 , 0.240 0.210 , 0.240	Depositor DCC
R_{free} test set	10416 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.277 for -k,-h,-l	Xtriage
Reported twinning fraction	0.749 for H, K, L 0.251 for -K, -H, -L	Depositor
Outliers	0 of 207034 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19260	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, GOL, ACT

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	0.73	0/1524	0.96	1/2071 (0.0%)
1	B	0.73	0/1487	0.94	3/2019 (0.1%)
1	C	0.65	0/1525	0.94	2/2072 (0.1%)
1	D	0.76	0/1558	0.95	3/2112 (0.1%)
1	E	0.68	0/1443	0.96	2/1958 (0.1%)
1	F	0.70	0/1515	0.95	2/2054 (0.1%)
1	G	0.71	0/1554	0.93	3/2113 (0.1%)
1	H	0.69	0/1467	0.97	2/1991 (0.1%)
1	I	0.69	0/1529	0.97	3/2075 (0.1%)
1	J	0.65	0/1538	0.92	4/2089 (0.2%)
1	K	0.64	0/1420	0.92	2/1925 (0.1%)
1	L	0.67	0/1498	0.94	3/2037 (0.1%)
All	All	0.69	0/18058	0.95	30/24516 (0.1%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	66	ASN	N-CA-C	9.07	124.00	113.38
1	I	146	LYS	N-CA-C	-8.62	101.22	112.68
1	L	66	ASN	N-CA-C	8.50	123.23	112.86
1	A	66	ASN	N-CA-C	8.35	123.14	113.38
1	C	23	ALA	N-CA-C	-7.58	102.95	111.14
1	J	146	LYS	N-CA-C	-6.76	105.03	113.55
1	I	66	ASN	N-CA-C	6.66	122.82	113.56
1	F	66	ASN	N-CA-C	6.47	122.55	113.56
1	D	66	ASN	N-CA-C	6.47	120.95	113.38
1	K	66	ASN	N-CA-C	6.46	122.54	113.56
1	B	186	SER	N-CA-C	-6.28	105.47	113.01
1	D	191	THR	CA-C-N	-6.22	113.97	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	191	THR	C-N-CA	-6.22	113.97	120.38
1	H	66	ASN	N-CA-C	6.16	120.59	113.38
1	K	195	GLY	N-CA-C	-6.15	107.37	114.69
1	B	66	ASN	N-CA-C	5.86	122.63	113.72
1	J	66[A]	ASN	N-CA-C	5.84	119.97	112.26
1	J	66[B]	ASN	N-CA-C	5.84	119.97	112.26
1	L	53	VAL	N-CA-C	-5.66	105.33	110.82
1	G	127	VAL	N-CA-C	5.60	116.02	108.17
1	H	81	ILE	N-CA-C	5.48	116.01	108.12
1	C	147	GLN	N-CA-C	5.43	116.78	108.52
1	I	42	SER	N-CA-C	-5.25	101.21	109.50
1	E	53	VAL	N-CA-C	-5.16	105.81	110.82
1	F	64	ARG	N-CA-C	-5.16	103.53	109.93
1	L	64	ARG	N-CA-C	-5.10	103.61	109.93
1	G	42	SER	N-CA-C	-5.09	101.46	109.50
1	E	186	SER	N-CA-C	-5.07	106.93	113.01
1	J	133	ASP	N-CA-C	5.06	117.00	108.96
1	B	199	ASP	N-CA-C	-5.02	99.16	107.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1490	0	1411	30	0
1	B	1453	0	1380	29	0
1	C	1491	0	1429	35	0
1	D	1524	0	1435	21	0
1	E	1409	0	1335	20	0
1	F	1482	0	1410	29	0
1	G	1520	0	1431	28	0
1	H	1434	0	1359	35	0
1	I	1494	0	1411	24	0
1	J	1503	0	1425	30	0
1	K	1389	0	1321	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1464	0	1385	29	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	D	4	0	3	0	0
2	F	4	0	3	1	0
2	G	4	0	3	0	0
2	H	4	0	3	2	0
2	I	4	0	3	0	0
3	A	7	0	10	0	0
3	D	14	0	20	0	0
3	J	7	0	10	0	0
4	A	6	0	8	0	0
4	H	6	0	8	0	0
5	A	144	0	0	5	0
5	B	141	0	0	7	0
5	C	128	0	0	10	0
5	D	153	0	0	6	0
5	E	102	0	0	0	0
5	F	119	0	0	8	0
5	G	139	0	0	6	0
5	H	149	0	0	15	0
5	I	138	0	0	4	0
5	J	108	0	0	4	0
5	K	109	0	0	4	0
5	L	109	0	0	12	0
All	All	19260	0	16809	319	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 (319) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:46[A]:THR:HG22	1:J:52:VAL:HG22	1.62	0.81
1:C:65[B]:PRO:HB3	5:C:409:HOH:O	1.79	0.81
1:L:153[B]:THR:HG22	1:L:157:THR:H	1.47	0.78
1:G:80[B]:LEU:HD21	1:G:87:LEU:HD11	1.67	0.77
1:F:145:LEU:HD21	1:F:148:PHE:CZ	2.20	0.77
1:H:79:VAL:HG13	5:H:514:HOH:O	1.85	0.75
1:K:46:THR:HG22	1:K:52:VAL:HG22	1.68	0.74
1:G:89[A]:PHE:HZ	5:H:406:HOH:O	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89[A]:PHE:HZ	5:H:491:HOH:O	1.72	0.73
1:G:164:VAL:HG22	1:G:170:ARG:HG2	1.69	0.72
1:C:46[A]:THR:HG22	1:C:52:VAL:HG22	1.70	0.72
1:B:89[A]:PHE:HZ	5:B:440:HOH:O	1.72	0.71
1:L:72[B]:MET:SD	5:L:338:HOH:O	2.47	0.71
1:L:153[B]:THR:HG21	5:L:374:HOH:O	1.90	0.71
1:B:108:ASN:ND2	5:B:519:HOH:O	2.24	0.70
1:L:71[B]:HIS:CD2	1:L:79:VAL:HG22	2.27	0.69
1:C:189:THR:HG22	5:C:357[B]:HOH:O	1.92	0.69
1:E:136:LEU:HD22	1:E:148[B]:PHE:CZ	2.28	0.69
1:I:183:VAL:HG11	1:I:187:LYS:HG3	1.74	0.68
1:L:189:THR:HG22	5:L:352[B]:HOH:O	1.94	0.68
1:E:136:LEU:HD13	1:E:148[B]:PHE:CE2	2.29	0.68
1:L:35[B]:ASN:OD1	1:L:35[B]:ASN:O	2.12	0.68
1:I:183:VAL:CG2	5:I:523:HOH:O	2.42	0.67
1:I:183:VAL:CG1	1:I:184:ASP:N	2.57	0.67
1:K:113:LEU:HD13	1:K:148:PHE:CZ	2.30	0.67
1:E:113:LEU:HD13	1:E:148[B]:PHE:CZ	2.30	0.67
1:C:177:SER:C	5:C:329:HOH:O	2.38	0.67
1:E:201[A]:GLN:NE2	1:F:135:GLU:OE2	2.29	0.66
1:H:108:ASN:HD21	2:H:301:ACT:H2	1.60	0.65
1:C:128[B]:LYS:HB2	1:C:128[B]:LYS:NZ	2.13	0.64
1:H:89[A]:PHE:CZ	5:H:491:HOH:O	2.48	0.64
1:H:46[B]:THR:HG22	5:H:475:HOH:O	1.98	0.64
1:L:52:VAL:HG11	1:L:55:GLU:HG3	1.78	0.64
1:K:176:LYS:O	1:K:177[B]:SER:HB3	1.97	0.63
1:D:162:THR:HG21	1:D:170[B]:ARG:HD2	1.80	0.63
1:E:191[A]:THR:HG23	1:E:191[A]:THR:O	1.96	0.63
1:I:183:VAL:HG12	1:I:184:ASP:N	2.11	0.63
1:C:65[B]:PRO:O	1:C:66[B]:ASN:HB2	1.98	0.62
1:G:137[B]:THR:HG23	5:G:445:HOH:O	2.00	0.62
1:H:187:LYS:HA	1:H:187:LYS:HZ3	1.64	0.62
1:C:52:VAL:HG11	1:C:55:GLU:HG3	1.82	0.62
1:B:145:LEU:HD13	1:B:148:PHE:CZ	2.35	0.61
1:B:191[A]:THR:HG23	5:B:486:HOH:O	2.00	0.60
1:J:110:PRO:HB3	1:J:148[B]:PHE:CE1	2.35	0.60
1:C:157:THR:HA	1:C:178:GLN:HE22	1.65	0.60
1:K:136:LEU:HD22	1:K:148:PHE:CZ	2.36	0.60
1:A:77:GLU:HG2	5:A:497:HOH:O	2.01	0.60
1:E:52:VAL:HG11	1:E:55:GLU:HG3	1.83	0.60
1:J:165[A]:GLU:HG2	1:J:166:GLN:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:TRP:CE2	1:A:187:LYS:HE2	2.36	0.59
1:C:136:LEU:HD12	1:C:136:LEU:N	2.17	0.59
1:F:65:PRO:HA	5:F:444:HOH:O	2.02	0.59
1:D:158:ILE:O	1:D:178:GLN:NE2	2.35	0.59
1:G:68:PHE:HE1	1:G:80[B]:LEU:HD22	1.67	0.59
1:J:65[A]:PRO:C	1:J:66[A]:ASN:OD1	2.46	0.59
1:K:148:PHE:HB2	1:K:162:THR:O	2.03	0.59
1:I:184:ASP:HB3	5:I:515:HOH:O	2.02	0.58
1:A:191[A]:THR:HG23	1:A:191[A]:THR:O	2.03	0.58
1:A:80:LEU:HD11	1:A:87:LEU:HD11	1.84	0.58
1:C:128[B]:LYS:HB2	1:C:128[B]:LYS:HZ2	1.66	0.58
1:K:65:PRO:HA	5:K:310:HOH:O	2.04	0.58
1:K:145:LEU:C	1:K:145:LEU:HD12	2.29	0.58
1:F:46[B]:THR:CG2	1:F:170:ARG:HB2	2.34	0.58
1:E:123[B]:LYS:HE2	5:I:514:HOH:O	2.04	0.57
1:J:22:ASP:N	5:J:490:HOH:O	2.36	0.57
1:F:136:LEU:N	1:F:136:LEU:HD12	2.19	0.57
1:L:94:VAL:HG21	5:L:360:HOH:O	2.04	0.57
1:F:46[B]:THR:HG22	5:F:426:HOH:O	2.04	0.56
1:F:199:ASP:OD1	1:F:201[A]:GLN:NE2	2.32	0.56
1:G:147:GLN:NE2	5:G:435:HOH:O	2.38	0.56
1:B:80:LEU:HD13	1:B:89[B]:PHE:CE2	2.41	0.56
1:F:89:PHE:HZ	5:F:451:HOH:O	1.87	0.56
1:J:54:GLN:NE2	1:J:75:PRO:CG	2.69	0.56
1:I:158:ILE:H	1:I:178:GLN:HE22	1.54	0.56
1:L:164:VAL:HG22	1:L:170:ARG:HG2	1.87	0.56
1:L:71[A]:HIS:NE2	1:L:73:THR:HG22	2.21	0.56
1:A:61:TRP:CD2	1:A:187:LYS:HE2	2.41	0.55
1:D:144:ASN:O	1:D:144:ASN:ND2	2.29	0.55
1:D:149:ALA:HB2	5:D:444:HOH:O	2.06	0.55
1:K:176:LYS:O	1:K:177[B]:SER:CB	2.55	0.55
1:L:136:LEU:N	1:L:136:LEU:HD12	2.22	0.55
1:D:89:PHE:HZ	5:D:417:HOH:O	1.90	0.55
1:L:35[B]:ASN:OD1	1:L:35[B]:ASN:C	2.49	0.54
1:E:46:THR:HG22	1:E:52:VAL:HG22	1.88	0.54
1:H:105:ALA:HB3	5:H:498:HOH:O	2.08	0.54
1:J:164:VAL:HG22	1:J:170:ARG:HG2	1.89	0.54
1:J:172:ALA:HB1	5:L:360:HOH:O	2.07	0.54
1:G:89[A]:PHE:CZ	5:H:406:HOH:O	2.51	0.54
1:F:185:ALA:HB1	5:F:446:HOH:O	2.07	0.54
1:J:162:THR:HG21	1:J:170:ARG:NH2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:PHE:HZ	5:C:316:HOH:O	1.90	0.54
1:E:71:HIS:CD2	1:E:79:VAL:HG22	2.42	0.54
1:L:43:GLN:HG2	1:L:44:ALA:N	2.22	0.54
1:G:78[A]:SER:HB3	1:H:52:VAL:HG23	1.90	0.54
1:H:68:PHE:CZ	5:H:543:HOH:O	2.60	0.54
1:K:71:HIS:CD2	1:K:79:VAL:HG22	2.43	0.54
1:C:178:GLN:N	5:C:329:HOH:O	2.41	0.53
1:B:193:PRO:HD2	1:B:196:VAL:HG21	1.91	0.53
1:J:46[B]:THR:HG22	5:J:461:HOH:O	2.07	0.53
1:K:124:GLN:HG2	5:K:385:HOH:O	2.09	0.53
1:J:52:VAL:HG23	1:L:78[B]:SER:OG	2.08	0.53
1:I:164:VAL:HG22	1:I:170:ARG:HG2	1.91	0.53
1:C:182:VAL:HG23	1:C:182:VAL:O	2.09	0.52
1:J:172:ALA:CB	5:L:360:HOH:O	2.56	0.52
1:J:54:GLN:NE2	1:J:75:PRO:HG3	2.24	0.52
1:L:158:ILE:H	1:L:178:GLN:HE22	1.56	0.52
1:B:91[B]:ASN:ND2	1:D:44:ALA:HB1	2.24	0.52
1:E:95:GLU:OE1	1:E:196:VAL:HG22	2.09	0.52
1:H:144:ASN:ND2	5:H:474[A]:HOH:O	2.42	0.52
1:L:46[B]:THR:HG21	1:L:170:ARG:NH1	2.24	0.52
1:H:187:LYS:HA	1:H:187:LYS:NZ	2.25	0.52
1:C:145:LEU:HD11	1:C:148:PHE:CZ	2.44	0.52
1:H:80:LEU:HD13	1:H:89[B]:PHE:CE2	2.45	0.52
1:A:138:PRO:HG3	1:A:145[A]:LEU:HD12	1.91	0.51
1:F:46[A]:THR:HG22	1:F:52:VAL:HG22	1.93	0.51
1:F:130[B]:LYS:O	1:F:130[B]:LYS:HD3	2.10	0.51
1:K:187:LYS:NZ	5:K:396:HOH:O	2.42	0.51
1:F:100:THR:HG22	1:F:201[A]:GLN:HB2	1.92	0.51
1:F:145:LEU:HD21	1:F:148:PHE:CE1	2.44	0.51
1:K:52:VAL:HG11	1:K:55:GLU:HG3	1.91	0.51
1:K:127:VAL:HG22	1:K:136:LEU:HG	1.91	0.51
1:G:40:SER:OG	1:G:176:LYS:HD2	2.10	0.51
1:H:191[A]:THR:HG23	1:H:191[A]:THR:O	2.10	0.51
1:F:127:VAL:HG22	1:F:136:LEU:HG	1.92	0.51
1:H:78[A]:SER:OG	1:H:89[A]:PHE:CE1	2.64	0.51
1:A:51:ALA:HB1	1:D:72:MET:HE1	1.92	0.51
1:K:70:TRP:CH2	1:K:72[A]:MET:HE2	2.46	0.51
1:H:109:THR:N	5:H:518:HOH:O	2.43	0.51
1:A:182:VAL:HG23	1:A:182:VAL:O	2.10	0.50
1:K:149:ALA:HB1	5:K:341:HOH:O	2.11	0.50
1:I:141:ALA:O	1:I:143:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65[B]:PRO:O	1:E:66[B]:ASN:HB2	2.11	0.50
1:E:191[A]:THR:O	1:E:191[A]:THR:CG2	2.60	0.50
1:A:127:VAL:HG22	1:A:136:LEU:HG	1.92	0.50
1:B:61:TRP:CZ3	1:B:187:LYS:HE2	2.47	0.50
1:C:106:THR:HG23	5:C:404:HOH:O	2.11	0.50
1:J:191[A]:THR:HG23	1:J:191[A]:THR:O	2.10	0.50
1:B:61:TRP:CH2	1:B:187:LYS:HE2	2.46	0.50
1:J:148[B]:PHE:CZ	1:J:150:ILE:HB	2.47	0.49
1:F:159:LYS:CD	5:F:501:HOH:O	2.60	0.49
1:C:145:LEU:HD11	1:C:148:PHE:CE1	2.48	0.49
1:G:46[A]:THR:HG21	1:I:89[A]:PHE:CZ	2.48	0.49
1:D:22:ASP:N	5:D:543:HOH:O	2.46	0.49
1:D:145:LEU:HD13	1:D:148:PHE:CZ	2.48	0.49
1:H:170:ARG:NH1	5:H:523:HOH:O	2.46	0.49
1:L:71[A]:HIS:CD2	1:L:73:THR:CG2	2.95	0.49
1:B:53:VAL:HG21	5:B:416:HOH:O	2.12	0.49
1:I:183:VAL:HG22	5:I:523:HOH:O	2.09	0.48
1:J:183:VAL:O	5:J:472:HOH:O	2.20	0.48
1:H:78[A]:SER:OG	1:H:89[A]:PHE:CZ	2.66	0.48
1:H:89[B]:PHE:O	1:H:97:ALA:HA	2.14	0.48
1:J:165[A]:GLU:CG	1:J:166:GLN:N	2.76	0.48
1:C:66[B]:ASN:N	5:C:359:HOH:O	2.46	0.48
1:G:46[B]:THR:HG21	5:G:461:HOH:O	2.13	0.48
1:A:85[B]:GLU:OE2	5:A:508:HOH:O	2.20	0.48
1:L:46[B]:THR:HG22	5:L:372:HOH:O	2.13	0.47
1:C:132:ASP:O	1:C:151:SER:HA	2.13	0.47
2:H:301:ACT:H3	1:I:48:SER:O	2.13	0.47
1:H:112:MET:SD	5:H:543:HOH:O	2.60	0.47
1:L:71[A]:HIS:CD2	1:L:73:THR:HG22	2.50	0.47
1:F:46[B]:THR:HG22	1:F:170:ARG:HB2	1.96	0.47
1:J:100:THR:HG22	1:J:201[B]:GLN:HB2	1.97	0.47
1:A:61:TRP:CZ2	1:A:187:LYS:HE2	2.50	0.47
1:A:183:VAL:HG22	1:A:184:ASP:N	2.30	0.47
1:C:46[A]:THR:CG2	1:C:52:VAL:HG22	2.42	0.47
1:D:170[B]:ARG:CZ	5:D:416:HOH:O	2.63	0.47
1:G:79:VAL:HG13	5:G:520:HOH:O	2.14	0.47
1:K:136:LEU:N	1:K:136:LEU:HD12	2.29	0.47
1:L:65:PRO:HA	5:L:308:HOH:O	2.15	0.47
1:B:64[B]:ARG:NH2	1:B:117:ASN:HB2	2.29	0.46
1:D:130[B]:LYS:NZ	1:D:130[B]:LYS:CB	2.78	0.46
1:G:89[A]:PHE:CZ	1:H:46[A]:THR:HG21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LEU:CD1	1:C:148:PHE:CE1	2.98	0.46
1:A:46[A]:THR:HG21	1:D:89:PHE:CZ	2.50	0.46
1:B:67:LEU:HD13	5:B:511:HOH:O	2.14	0.46
1:B:78[B]:SER:HB2	1:D:52:VAL:HG23	1.98	0.46
1:G:78[B]:SER:HB2	1:H:52:VAL:HG23	1.95	0.46
1:E:136:LEU:HD22	1:E:148[B]:PHE:HZ	1.79	0.46
1:K:191[A]:THR:HG23	1:K:191[A]:THR:O	2.14	0.46
1:B:191[A]:THR:HG23	1:B:191[A]:THR:O	2.15	0.46
1:D:46[B]:THR:HG22	5:D:418:HOH:O	2.14	0.46
1:C:52:VAL:HG11	1:C:55:GLU:CG	2.46	0.46
1:I:80:LEU:HD13	1:I:89[B]:PHE:CE2	2.51	0.46
1:I:193:PRO:HD2	1:I:196:VAL:HG21	1.97	0.46
1:A:77:GLU:CG	5:A:497:HOH:O	2.60	0.46
1:B:161:PHE:CE2	1:B:175:LEU:HD11	2.51	0.45
1:C:191[A]:THR:HG23	1:C:191[A]:THR:O	2.15	0.45
1:D:158:ILE:N	1:D:178:GLN:HE22	2.15	0.45
1:L:153[B]:THR:HG23	1:L:155:SER:H	1.81	0.45
1:I:38[B]:HIS:CE1	1:I:179:GLN:HB2	2.51	0.45
1:J:65[A]:PRO:O	1:J:66[A]:ASN:OD1	2.35	0.45
1:A:145[A]:LEU:HD13	1:A:146:LYS:N	2.32	0.45
1:F:116:ARG:HA	2:F:301:ACT:H2	1.98	0.45
1:B:70:TRP:CH2	1:B:72[A]:MET:HE2	2.52	0.45
1:C:157:THR:HA	1:C:178:GLN:NE2	2.32	0.45
1:F:145:LEU:CD2	1:F:148:PHE:CE1	3.00	0.45
1:C:89:PHE:O	1:C:97:ALA:HA	2.17	0.45
1:J:136:LEU:HD12	1:J:136:LEU:N	2.32	0.45
1:B:63:LYS:HD2	1:B:67:LEU:HD12	1.97	0.45
1:B:38[B]:HIS:HB3	1:B:61:TRP:CD1	2.52	0.44
1:E:91:ASN:OD1	1:E:94:VAL:HG22	2.17	0.44
1:F:145:LEU:CD1	1:F:145:LEU:C	2.91	0.44
1:K:187:LYS:HE3	1:K:187:LYS:HA	1.99	0.44
1:L:60:LEU:HD12	1:L:60:LEU:O	2.18	0.44
1:B:95:GLU:OE1	1:B:196:VAL:HG22	2.18	0.44
1:G:51:ALA:HB1	1:I:72[A]:MET:HE1	1.99	0.44
1:J:100:THR:HG22	1:J:201[A]:GLN:HB2	2.00	0.44
1:J:127:VAL:HG22	1:J:136:LEU:HG	1.99	0.44
1:K:61:TRP:CD2	1:K:187:LYS:HD3	2.53	0.44
1:F:145:LEU:CD2	1:F:148:PHE:CZ	2.97	0.44
1:B:89[A]:PHE:CZ	5:B:440:HOH:O	2.55	0.44
1:B:111:PHE:O	1:B:115:THR:HG23	2.18	0.44
1:G:135[A]:GLU:HG3	1:G:147:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:TRP:CZ2	1:K:72[A]:MET:HE2	2.53	0.43
1:A:57:GLU:HG2	1:A:74[B]:SER:HB3	2.00	0.43
1:A:164:VAL:HG22	1:A:170:ARG:HG2	2.00	0.43
1:B:35:ASN:HB3	1:B:64[B]:ARG:HB2	2.00	0.43
1:F:94:VAL:HG23	1:F:96[B]:GLN:HG2	2.00	0.43
1:H:100:THR:HG22	1:H:201[A]:GLN:HB2	2.00	0.43
1:C:106:THR:CG2	5:C:404:HOH:O	2.64	0.43
1:E:89:PHE:O	1:E:97:ALA:HA	2.19	0.43
1:H:116:ARG:NH1	5:H:498:HOH:O	2.50	0.43
1:H:116:ARG:O	1:H:117:ASN:C	2.61	0.43
1:B:102:LEU:HD23	5:B:509:HOH:O	2.19	0.43
1:G:52:VAL:HG23	1:I:78:SER:HB2	2.00	0.43
1:H:176:LYS:O	1:H:177:SER:C	2.62	0.43
1:K:113:LEU:CD1	1:K:148:PHE:CZ	2.99	0.43
1:A:78:SER:HB2	1:B:52:VAL:HG23	2.01	0.43
1:G:176:LYS:O	1:G:177:SER:C	2.62	0.43
1:H:52:VAL:HG11	1:H:55:GLU:HG3	2.01	0.43
1:A:52:VAL:HG23	1:D:78:SER:HB2	2.00	0.43
1:A:183:VAL:HG22	1:A:184:ASP:H	1.83	0.43
1:C:26:ASP:OD1	5:C:398[B]:HOH:O	2.21	0.43
1:C:183:VAL:HG22	1:C:184:ASP:N	2.33	0.43
1:D:52:VAL:HG11	1:D:55:GLU:HG3	2.00	0.43
1:G:145:LEU:N	1:G:145:LEU:HD23	2.34	0.43
1:K:71:HIS:CE1	1:K:73:THR:HG22	2.54	0.43
1:E:153:THR:HB	1:E:154:PRO:HD2	2.00	0.43
1:B:64[B]:ARG:NH2	1:B:117:ASN:CB	2.82	0.42
1:C:145:LEU:CD1	1:C:148:PHE:CZ	3.02	0.42
1:F:135:GLU:C	1:F:136:LEU:HD12	2.44	0.42
1:G:150:ILE:O	1:G:150:ILE:HG23	2.19	0.42
1:A:46[B]:THR:HG22	5:A:425:HOH:O	2.19	0.42
1:J:54:GLN:NE2	1:J:75:PRO:HG2	2.33	0.42
1:J:191[A]:THR:HG22	5:J:455:HOH:O	2.19	0.42
1:L:46[B]:THR:HG23	5:L:346:HOH:O	2.19	0.42
1:C:100:THR:HG22	1:C:201[A]:GLN:HB2	2.01	0.42
1:E:162:THR:HG21	1:E:170:ARG:NH2	2.33	0.42
1:H:95:GLU:HA	1:H:95:GLU:OE1	2.19	0.42
1:A:147:GLN:HB2	5:A:503:HOH:O	2.18	0.42
1:F:110:PRO:HD3	1:F:148:PHE:CE1	2.54	0.42
1:K:91:ASN:OD1	1:K:91:ASN:C	2.62	0.42
1:B:80:LEU:HD13	1:B:89[B]:PHE:CD2	2.54	0.42
1:F:46[A]:THR:HG22	1:F:52:VAL:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89[A]:PHE:O	1:H:97:ALA:HA	2.19	0.42
1:H:164:VAL:HG22	1:H:170:ARG:HG2	2.02	0.42
1:A:110:PRO:HD3	1:A:148:PHE:CE1	2.55	0.42
1:C:135:GLU:C	1:C:136:LEU:HD12	2.45	0.42
1:H:108:ASN:C	5:H:518:HOH:O	2.62	0.42
1:J:89:PHE:O	1:J:97:ALA:HA	2.19	0.42
1:L:116:ARG:O	1:L:117:ASN:C	2.62	0.42
1:K:43:GLN:HG2	1:K:44:ALA:N	2.34	0.42
1:A:145[A]:LEU:HD13	1:A:145[A]:LEU:C	2.45	0.42
1:F:64:ARG:HA	1:F:65:PRO:HA	1.80	0.42
1:F:100:THR:HG22	1:F:201[B]:GLN:HB2	2.00	0.42
1:G:80[B]:LEU:CD2	1:G:80[B]:LEU:C	2.93	0.42
1:G:182:VAL:HG23	1:G:182:VAL:O	2.20	0.42
1:H:43:GLN:HG2	1:H:44:ALA:N	2.34	0.42
1:B:43:GLN:HG2	1:B:44:ALA:N	2.34	0.41
1:D:176:LYS:O	1:D:177:SER:C	2.63	0.41
1:F:199:ASP:CG	1:F:201[A]:GLN:HE21	2.24	0.41
1:H:162:THR:HG21	1:H:170:ARG:NH1	2.35	0.41
1:C:100:THR:HG22	1:C:201[B]:GLN:HB2	2.01	0.41
1:C:110:PRO:HG3	1:C:148:PHE:CD1	2.54	0.41
1:C:110:PRO:HD3	1:C:148:PHE:CE1	2.55	0.41
1:G:147:GLN:CG	1:G:148:PHE:N	2.83	0.41
1:I:43:GLN:HG2	1:I:44:ALA:N	2.35	0.41
1:K:52:VAL:HG11	1:K:55:GLU:CG	2.49	0.41
1:L:46[A]:THR:HG22	1:L:52:VAL:HG22	2.03	0.41
1:J:111:PHE:O	1:J:115:THR:HG23	2.21	0.41
1:A:24:SER:O	1:A:28:GLN:HG3	2.21	0.41
1:A:191[A]:THR:O	1:A:191[A]:THR:CG2	2.68	0.41
1:B:89[B]:PHE:O	1:B:97:ALA:HA	2.20	0.41
1:F:152:VAL:CG2	5:F:474:HOH:O	2.67	0.41
1:G:146:LYS:HD2	5:G:524:HOH:O	2.19	0.41
1:J:145:LEU:HD12	1:J:147:GLN:CA	2.49	0.41
1:G:127:VAL:HG22	1:G:136:LEU:HG	2.03	0.41
1:A:100:THR:HG22	1:A:201[A]:GLN:HB2	2.03	0.41
1:K:89:PHE:O	1:K:97:ALA:HA	2.20	0.41
1:H:78[B]:SER:HB3	1:I:52:VAL:HG23	2.02	0.41
1:I:64:ARG:HA	1:I:65:PRO:HA	1.82	0.41
1:I:194:LYS:CD	1:K:59[B]:GLU:HG3	2.51	0.41
1:A:61:TRP:CE3	1:A:187:LYS:HE2	2.55	0.41
1:C:72[A]:MET:SD	5:C:351:HOH:O	2.63	0.41
1:D:71:HIS:CE1	1:D:73:THR:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:31:LEU:HD22	1:I:114[B]:ILE:HD12	2.02	0.41
1:I:194:LYS:HD3	1:K:59[B]:GLU:HG3	2.02	0.41
1:J:72[B]:MET:HE1	1:K:51:ALA:HB1	2.03	0.41
1:L:25[A]:THR:HG23	5:L:393:HOH:O	2.20	0.41
1:A:136:LEU:HD12	1:A:136:LEU:N	2.35	0.41
1:C:64[A]:ARG:HA	1:C:65[A]:PRO:HA	1.50	0.41
1:E:136:LEU:HD12	1:E:136:LEU:N	2.35	0.41
1:G:28:GLN:HG2	1:G:122:TRP:CD1	2.56	0.41
1:B:89[A]:PHE:CZ	1:D:46[A]:THR:HG21	2.56	0.40
1:E:111:PHE:O	1:E:115:THR:HG23	2.21	0.40
1:G:36[B]:SER:OG	1:G:63:LYS:HG3	2.22	0.40
1:J:162:THR:HG21	1:J:170:ARG:CZ	2.51	0.40
1:L:22:ASP:N	5:L:355:HOH:O	2.54	0.40
1:A:145[A]:LEU:HD13	1:A:146:LYS:C	2.47	0.40
1:E:45:VAL:HG21	5:F:511:HOH:O	2.22	0.40
1:F:159:LYS:HD2	5:F:501:HOH:O	2.21	0.40
1:L:72[A]:MET:O	1:L:77:GLU:HA	2.21	0.40
1:D:165[A]:GLU:OE1	5:D:516:HOH:O	2.22	0.40
1:H:68:PHE:CE2	5:H:543:HOH:O	2.57	0.40
1:I:183:VAL:CG1	1:I:184:ASP:H	2.34	0.40
1:G:146:LYS:HE3	5:G:435:HOH:O	2.20	0.40
1:H:78[A]:SER:HB2	1:I:52:VAL:HG23	2.03	0.40
1:J:118[B]:ASN:OD1	1:J:118[B]:ASN:C	2.63	0.40
1:L:85:GLU:HB2	5:L:322:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	184/184 (100%)	180 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	177/184 (96%)	174 (98%)	3 (2%)	0	100	100
1	C	185/184 (100%)	179 (97%)	6 (3%)	0	100	100
1	D	189/184 (103%)	185 (98%)	4 (2%)	0	100	100
1	E	172/184 (94%)	166 (96%)	6 (4%)	0	100	100
1	F	184/184 (100%)	176 (96%)	8 (4%)	0	100	100
1	G	190/184 (103%)	185 (97%)	5 (3%)	0	100	100
1	H	176/184 (96%)	173 (98%)	3 (2%)	0	100	100
1	I	186/184 (101%)	181 (97%)	5 (3%)	0	100	100
1	J	186/184 (101%)	182 (98%)	2 (1%)	2 (1%)	11	3
1	K	169/184 (92%)	165 (98%)	4 (2%)	0	100	100
1	L	182/184 (99%)	180 (99%)	2 (1%)	0	100	100
All	All	2180/2208 (99%)	2126 (98%)	52 (2%)	2 (0%)	100	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	65[A]	PRO
1	J	65[B]	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/161 (105%)	169 (100%)	0	100	100
1	B	163/161 (101%)	163 (100%)	0	100	100
1	C	169/161 (105%)	169 (100%)	0	100	100
1	D	172/161 (107%)	171 (99%)	1 (1%)	78	72
1	E	158/161 (98%)	158 (100%)	0	100	100
1	F	168/161 (104%)	166 (99%)	2 (1%)	63	51
1	G	173/161 (108%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	161/161 (100%)	160 (99%)	1 (1%)	78	72
1	I	168/161 (104%)	168 (100%)	0	100	100
1	J	170/161 (106%)	170 (100%)	0	100	100
1	K	155/161 (96%)	154 (99%)	1 (1%)	78	72
1	L	166/161 (103%)	166 (100%)	0	100	100
All	All	1992/1932 (103%)	1987 (100%)	5 (0%)	86	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	144	ASN
1	F	145	LEU
1	F	187	LYS
1	H	187	LYS
1	K	187	LYS

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

Mol	Chain	Res	Type
1	A	28	GLN
1	B	28	GLN
1	D	43	GLN
1	D	178	GLN
1	E	28	GLN
1	E	38	HIS
1	E	43	GLN
1	E	96	GLN
1	F	43	GLN
1	F	129	GLN
1	G	28	GLN
1	I	28	GLN
1	I	29	ASN
1	I	129	GLN
1	K	28	GLN
1	L	28	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	B	301	-	3,3,3	0.71	0	3,3,3	1.38	0
2	ACT	A	301	-	3,3,3	0.85	0	3,3,3	1.16	0
2	ACT	I	301	-	3,3,3	0.88	0	3,3,3	1.40	0
3	PEG	D	302[B]	-	6,6,6	0.42	0	5,5,5	0.35	0
3	PEG	A	302	-	6,6,6	0.45	0	5,5,5	0.24	0
3	PEG	J	301	-	6,6,6	0.42	0	5,5,5	0.33	0
3	PEG	D	302[A]	-	6,6,6	0.46	0	5,5,5	0.25	0
2	ACT	F	301	-	3,3,3	0.72	0	3,3,3	1.32	0
4	GOL	H	302	-	5,5,5	0.34	0	5,5,5	0.36	0
2	ACT	H	301	-	3,3,3	0.79	0	3,3,3	1.25	0
2	ACT	D	301	-	3,3,3	0.83	0	3,3,3	1.42	0
4	GOL	A	303	-	5,5,5	0.43	0	5,5,5	0.15	0
2	ACT	G	301	-	3,3,3	0.83	0	3,3,3	1.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	D	302[B]	-	-	2/4/4/4	-
3	PEG	A	302	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	J	301	-	-	3/4/4/4	-
3	PEG	D	302[A]	-	-	4/4/4/4	-
4	GOL	H	302	-	-	3/4/4/4	-
4	GOL	A	303	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	302	GOL	C1-C2-C3-O3
4	H	302	GOL	O2-C2-C3-O3
3	A	302	PEG	O1-C1-C2-O2
3	A	302	PEG	O2-C3-C4-O4
3	D	302[A]	PEG	O2-C3-C4-O4
3	D	302[A]	PEG	O1-C1-C2-O2
3	J	301	PEG	C1-C2-O2-C3
3	D	302[A]	PEG	C4-C3-O2-C2
3	D	302[B]	PEG	O2-C3-C4-O4
3	J	301	PEG	O2-C3-C4-O4
3	D	302[B]	PEG	C4-C3-O2-C2
3	A	302	PEG	C4-C3-O2-C2
3	J	301	PEG	C4-C3-O2-C2
4	H	302	GOL	O1-C1-C2-C3
3	D	302[A]	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	ACT	1	0
2	H	301	ACT	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	177/184 (96%)	-0.76	0 100 100	11, 24, 38, 51	12 (6%)
1	B	169/184 (91%)	-0.73	0 100 100	9, 24, 33, 40	14 (8%)
1	C	177/184 (96%)	-0.60	0 100 100	9, 27, 44, 48	12 (6%)
1	D	179/184 (97%)	-0.76	0 100 100	10, 23, 39, 47	14 (7%)
1	E	169/184 (91%)	-0.67	0 100 100	12, 27, 40, 48	9 (5%)
1	F	177/184 (96%)	-0.62	0 100 100	10, 27, 42, 46	11 (6%)
1	G	179/184 (97%)	-0.71	0 100 100	9, 25, 41, 52	15 (8%)
1	H	172/184 (93%)	-0.74	0 100 100	11, 24, 36, 42	10 (5%)
1	I	180/184 (97%)	-0.74	0 100 100	10, 25, 41, 48	10 (5%)
1	J	177/184 (96%)	-0.58	0 100 100	12, 28, 45, 50	13 (7%)
1	K	171/184 (92%)	-0.60	0 100 100	12, 30, 43, 52	5 (2%)
1	L	176/184 (95%)	-0.58	0 100 100	11, 29, 44, 49	10 (5%)
All	All	2103/2208 (95%)	-0.68	0 100 100	9, 26, 42, 52	135 (6%)

There are no RSRZ outliers to report.

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
2	ACT	A	301	4/4	0.90	0.08	36,37,37,38	0
2	ACT	I	301	4/4	0.94	0.08	38,38,38,38	0
3	PEG	A	302	7/7	0.95	0.07	32,40,44,44	0
3	PEG	J	301	7/7	0.96	0.07	42,43,43,44	0
4	GOL	H	302	6/6	0.96	0.06	47,48,48,48	0
2	ACT	G	301	4/4	0.97	0.08	42,42,43,43	0
3	PEG	D	302[A]	7/7	0.97	0.06	31,38,39,40	7
3	PEG	D	302[B]	7/7	0.97	0.06	40,43,44,44	7
2	ACT	H	301	4/4	0.97	0.07	37,37,38,39	0
4	GOL	A	303	6/6	0.97	0.06	31,36,37,39	0
2	ACT	F	301	4/4	0.97	0.06	39,39,40,41	0
2	ACT	B	301	4/4	0.98	0.06	38,38,38,39	0
2	ACT	D	301	4/4	0.98	0.06	44,45,45,45	0

6.5 Other polymers

There are no such residues in this entry.