



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:59 PM UTC

PDB ID : 5CER / pdb_00005cer
Title : Bd0816 Predatory Endopeptidase from Bdellovibrio bacteriovorus in complex with immunity protein Bd3460
Authors : Lovering, A.L.; Cadby, I.T.; Lambert, C.; Sockett, R.E.
Deposited on : 2015-07-07
Resolution : 2.48 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

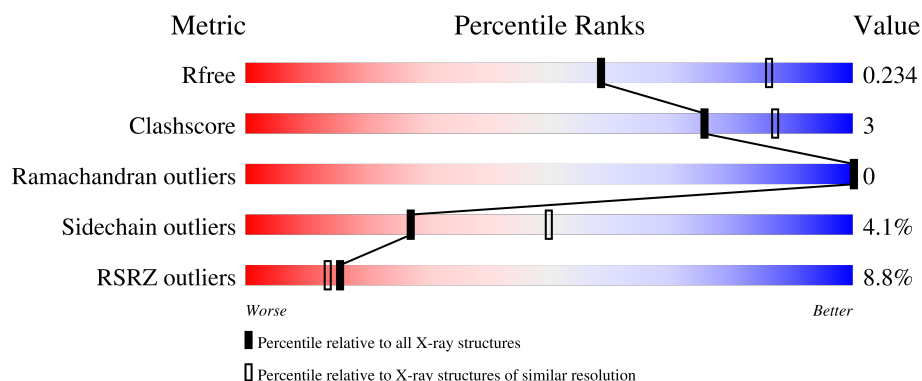
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	401	5% 90% 9%
1	C	401	17% 91% 7%
1	E	401	6% 89% 9%
1	G	401	14% 89% 9%
1	I	401	9% 90% 9%

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Mol	Chain	Length	Quality of chain
1	K	401	9% 88% 9% .
2	B	193	5% 94% 6%
2	D	193	5% 96% ..
2	F	193	7% 95% 5%
2	H	193	5% 92% 8%
2	J	193	10% 92% 6% ..
2	L	193	6% 92% 6% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28724 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 Bd0816.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3124	1970	536	604	14			
1	C	401	Total	C	N	O	S	0	0	0
			3124	1970	536	604	14			
1	E	401	Total	C	N	O	S	0	0	0
			3124	1970	536	604	14			
1	G	399	Total	C	N	O	S	0	0	0
			3110	1962	534	600	14			
1	I	401	Total	C	N	O	S	0	0	0
			3124	1970	536	604	14			
1	K	400	Total	C	N	O	S	0	1	0
			3124	1971	535	603	15			

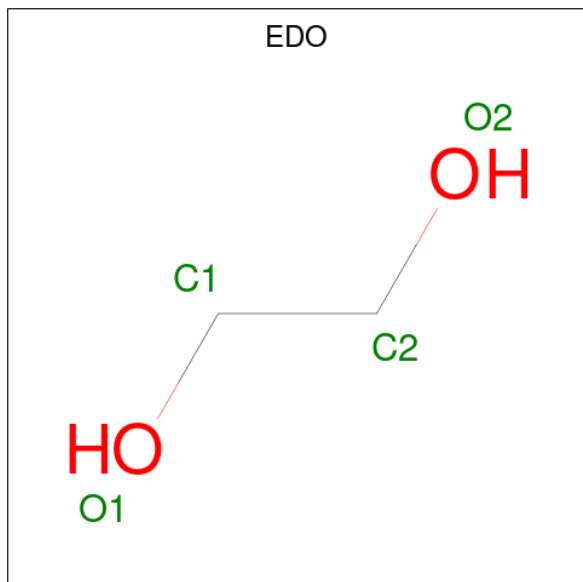
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	LYS	engineered mutation	UNP Q6MPN2
A	58	ALA	SER	engineered mutation	UNP Q6MPN2
C	26	MET	LYS	engineered mutation	UNP Q6MPN2
C	58	ALA	SER	engineered mutation	UNP Q6MPN2
E	26	MET	LYS	engineered mutation	UNP Q6MPN2
E	58	ALA	SER	engineered mutation	UNP Q6MPN2
G	26	MET	LYS	engineered mutation	UNP Q6MPN2
G	58	ALA	SER	engineered mutation	UNP Q6MPN2
I	26	MET	LYS	engineered mutation	UNP Q6MPN2
I	58	ALA	SER	engineered mutation	UNP Q6MPN2
K	26	MET	LYS	engineered mutation	UNP Q6MPN2
K	58	ALA	SER	engineered mutation	UNP Q6MPN2

- Molecule 2 is a protein called Bd3460.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	0	0
			1439	897	250	288	4			
2	D	193	Total	C	N	O	S	0	0	0
			1439	897	250	288	4			
2	F	193	Total	C	N	O	S	0	0	0
			1439	897	250	288	4			
2	H	193	Total	C	N	O	S	0	0	0
			1439	897	250	288	4			
2	J	193	Total	C	N	O	S	0	0	0
			1439	897	250	288	4			
2	L	193	Total	C	N	O	S	0	0	0
			1439	897	250	288	4			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	181	Total	O	0	0
			181	181		
4	B	93	Total	O	0	0
			93	93		
4	C	141	Total	O	0	0
			141	141		

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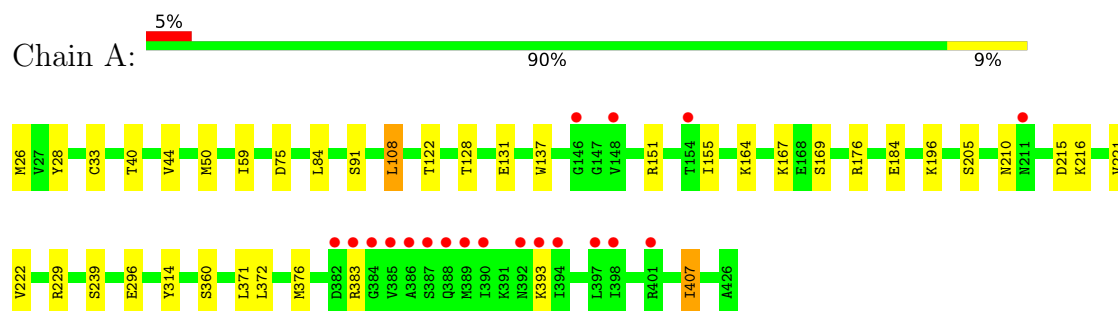
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	94	Total 94	O 94	0	0
4	E	141	Total 141	O 141	0	0
4	F	77	Total 77	O 77	0	0
4	G	112	Total 112	O 112	0	0
4	H	84	Total 84	O 84	0	0
4	I	131	Total 131	O 131	0	0
4	J	69	Total 69	O 69	0	0
4	K	136	Total 136	O 136	0	0
4	L	97	Total 97	O 97	0	0

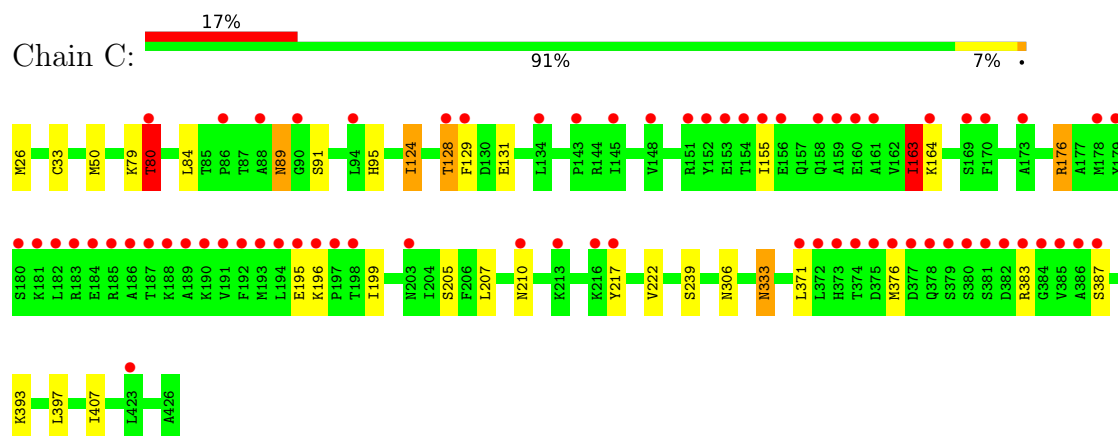
3 Residue-property plots [i](#)

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.

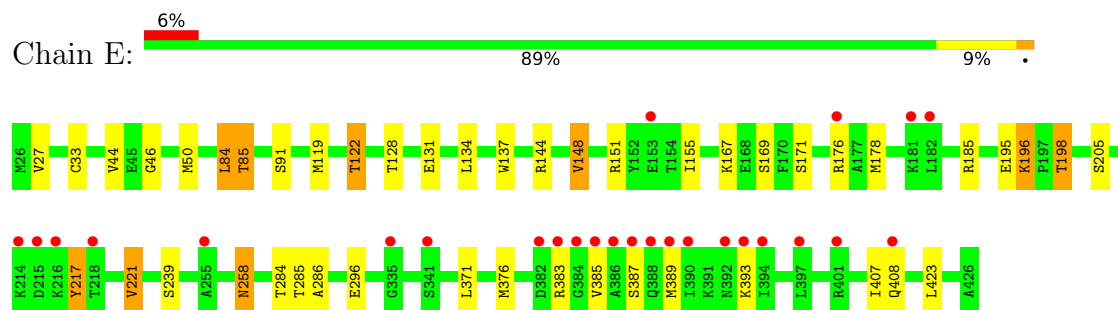
• Molecule 1: Bd0816



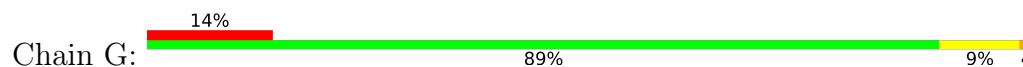
• Molecule 1: Bd0816

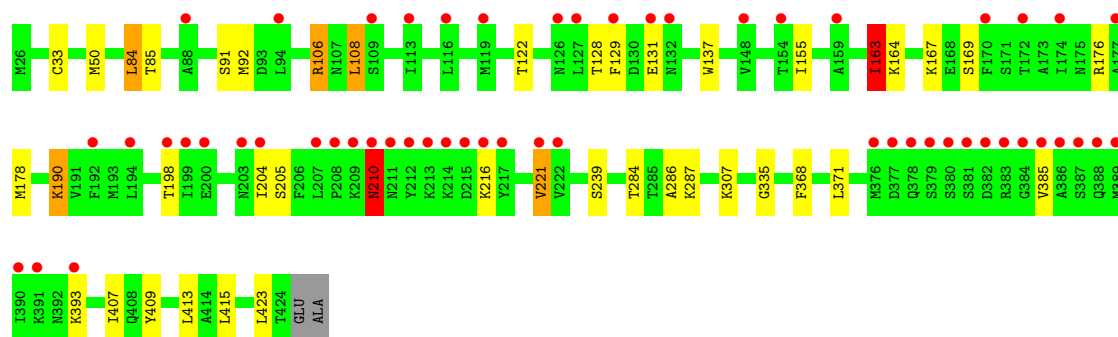


• Molecule 1: Bd0816

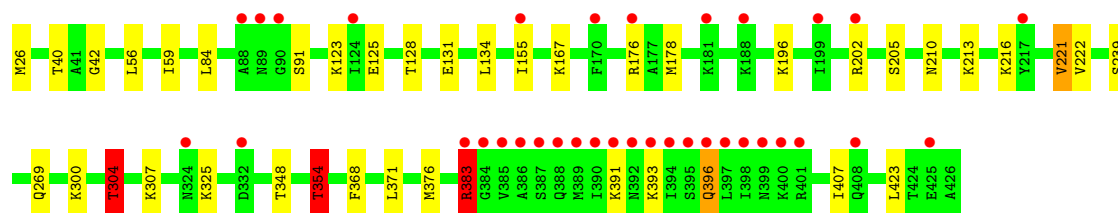
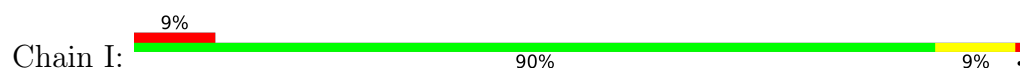


• Molecule 1: Bd0816

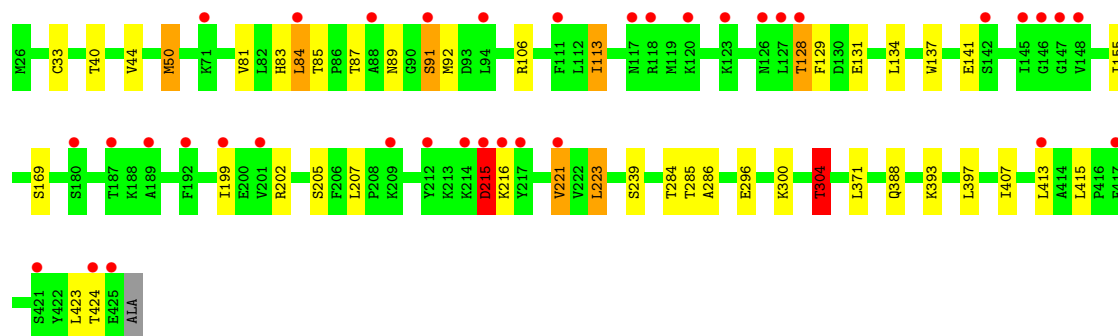




• Molecule 1: Bd0816



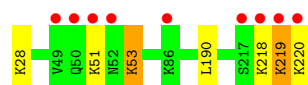
• Molecule 1: Bd0816



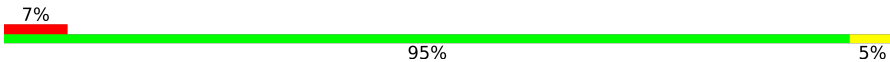
• Molecule 2: Bd3460



• Molecule 2: Bd3460

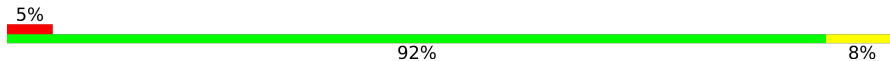


● Molecule 2: Bd3460

Chain F: 

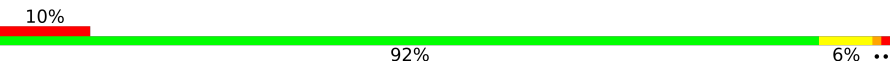


● Molecule 2: Bd3460

Chain H: 

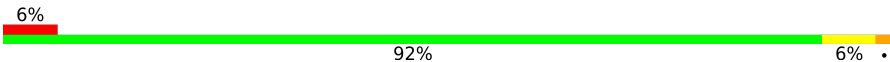


● Molecule 2: Bd3460

Chain J: 



● Molecule 2: Bd3460

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	237.45Å 212.32Å 90.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.48 100.00 – 2.48	Depositor EDS
% Data completeness (in resolution range)	98.8 (100.00-2.48) 98.8 (100.00-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.215 , 0.249 (Not available) , 0.234	Depositor DCC
R_{free} test set	7978 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	28724	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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: EDO

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	0.95	4/3176 (0.1%)	0.97	0/4287
1	C	0.96	2/3176 (0.1%)	1.01	5/4287 (0.1%)
1	E	0.98	3/3176 (0.1%)	1.04	14/4287 (0.3%)
1	G	0.85	0/3162	1.00	5/4268 (0.1%)
1	I	0.96	1/3176 (0.0%)	1.01	6/4287 (0.1%)
1	K	0.92	1/3179 (0.0%)	1.01	5/4290 (0.1%)
2	B	0.92	1/1447 (0.1%)	0.98	4/1940 (0.2%)
2	D	0.89	0/1447	1.01	2/1940 (0.1%)
2	F	0.87	0/1447	0.95	1/1940 (0.1%)
2	H	0.90	0/1447	0.99	2/1940 (0.1%)
2	J	0.88	1/1447 (0.1%)	1.02	4/1940 (0.2%)
2	L	0.89	1/1447 (0.1%)	0.98	0/1940
All	All	0.92	14/27727 (0.1%)	1.00	48/37346 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
1	K	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	333	ASN	C-N	11.26	1.48	1.33
2	L	185	LYS	CA-CB	7.00	1.64	1.53
1	A	407	ILE	CA-C	6.79	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	GLU	CA-CB	6.72	1.63	1.53
1	E	217	TYR	CA-CB	6.50	1.62	1.53
1	K	113	ILE	CA-CB	6.35	1.61	1.54
2	B	77	ASP	CA-CB	6.26	1.63	1.53
1	E	171	SER	CA-CB	6.18	1.64	1.53
1	C	80	THR	CA-CB	6.00	1.62	1.53
1	E	46	GLY	C-O	-5.81	1.19	1.23
2	J	53	LYS	CA-C	5.52	1.60	1.52
1	A	407	ILE	CB-CG1	5.36	1.64	1.53
1	A	407	ILE	CA-CB	5.26	1.61	1.54
1	I	383	ARG	CD-NE	5.21	1.53	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	148	VAL	CB-CA-C	9.10	121.72	111.08
1	E	185	ARG	CG-CD-NE	9.04	131.89	112.00
1	K	113	ILE	CA-CB-CG1	8.50	124.85	110.40
1	G	163	ILE	CA-CB-CG1	8.25	124.42	110.40
1	I	383	ARG	CG-CD-NE	8.23	130.11	112.00
1	C	163	ILE	CA-CB-CG1	8.09	124.16	110.40
2	J	86	LYS	CA-CB-CG	7.36	128.81	114.10
2	H	196	LYS	CG-CD-CE	6.95	127.29	111.30
2	D	51	LYS	CB-CA-C	-6.89	97.08	110.46
2	J	51	LYS	CB-CA-C	-6.84	97.19	110.46
1	C	124	ILE	CG1-CB-CG2	-6.72	90.53	110.70
1	G	190	LYS	CA-CB-CG	6.34	126.78	114.10
1	I	354	THR	N-CA-CB	-6.32	99.78	111.53
1	K	223	LEU	CB-CG-CD2	-6.32	91.74	110.70
2	J	51	LYS	CG-CD-CE	6.23	125.62	111.30
1	I	396	GLN	CA-CB-CG	6.22	126.53	114.10
2	D	51	LYS	CG-CD-CE	6.16	125.46	111.30
1	E	185	ARG	CD-NE-CZ	-6.12	115.83	124.40
1	E	148	VAL	N-CA-CB	6.01	117.68	110.95
2	J	53	LYS	CB-CA-C	5.93	121.59	109.55
1	E	178	MET	CG-SD-CE	5.93	113.94	100.90
1	C	124	ILE	CB-CG1-CD1	5.90	126.19	113.80
1	E	258	ASN	CB-CA-C	-5.83	101.11	110.79
1	E	195	GLU	CA-C-N	5.79	135.93	121.80
1	E	195	GLU	C-N-CA	5.79	135.93	121.80
1	K	202	ARG	CA-CB-CG	5.78	125.65	114.10
1	K	215	ASP	CB-CA-C	5.71	121.13	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	196	LYS	CB-CA-C	-5.65	99.05	110.17
1	E	195	GLU	O-C-N	5.62	128.08	122.12
2	B	77	ASP	CB-CA-C	5.58	119.65	110.88
1	E	122	THR	N-CA-CB	5.51	118.75	110.65
1	C	176	ARG	CB-CG-CD	5.49	123.94	111.30
2	B	181	ASP	CB-CA-C	-5.48	100.15	110.67
2	B	51	LYS	CG-CD-CE	-5.45	98.76	111.30
1	G	210	ASN	N-CA-C	5.44	117.91	111.33
2	F	51	LYS	CG-CD-CE	-5.41	98.86	111.30
1	E	387	SER	CB-CA-C	-5.38	102.43	110.88
2	H	51	LYS	CG-CD-CE	-5.36	98.97	111.30
1	I	304	THR	CB-CA-C	5.36	120.95	110.67
1	G	106	ARG	CG-CD-NE	-5.35	100.23	112.00
1	C	387	SER	CB-CA-C	-5.33	102.51	110.88
1	E	85	THR	CB-CA-C	5.30	116.58	109.42
1	I	325	LYS	N-CA-C	5.29	117.96	111.82
2	B	53	LYS	CB-CG-CD	5.21	123.28	111.30
1	G	163	ILE	CB-CG1-CD1	5.19	124.70	113.80
1	K	304	THR	CB-CA-C	5.13	120.52	110.67
1	E	196	LYS	N-CA-CB	-5.07	101.34	110.37
1	I	269	GLN	N-CA-C	5.07	118.23	111.75

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	333	ASN	Mainchain
1	E	196	LYS	Peptide
1	K	424	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3124	0	3148	19	0
1	C	3124	0	3148	23	0
1	E	3124	0	3148	25	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3110	0	3137	25	0
1	I	3124	0	3148	26	1
1	K	3124	0	3152	31	0
2	B	1439	0	1499	3	0
2	D	1439	0	1499	3	1
2	F	1439	0	1499	3	0
2	H	1439	0	1499	8	0
2	J	1439	0	1499	7	1
2	L	1439	0	1499	7	0
3	I	4	0	6	3	0
4	A	181	0	0	1	0
4	B	93	0	0	0	0
4	C	141	0	0	6	0
4	D	94	0	0	1	0
4	E	141	0	0	1	0
4	F	77	0	0	0	0
4	G	112	0	0	0	0
4	H	84	0	0	1	0
4	I	131	0	0	1	0
4	J	69	0	0	0	0
4	K	136	0	0	1	0
4	L	97	0	0	0	0
All	All	28724	0	27881	168	2

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 3.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:385:VAL:HG12	1:E:389:MET:CE	1.78	1.13
1:I:376:MET:HE3	1:I:383:ARG:NH1	1.70	1.07
1:E:385:VAL:HG12	1:E:389:MET:HE3	1.54	0.89
1:A:75:ASP:OD1	1:A:229:ARG:NH1	2.08	0.85
1:G:84:LEU:HB3	1:G:92:MET:HE2	1.63	0.79
1:K:84:LEU:HB3	1:K:92:MET:HE2	1.63	0.79
1:I:376:MET:HE1	1:I:383:ARG:HB2	1.66	0.78
1:E:376:MET:HE1	1:E:383:ARG:HB2	1.65	0.78
1:A:376:MET:HE1	1:A:383:ARG:HB2	1.66	0.77
1:I:376:MET:CE	1:I:383:ARG:NH1	2.46	0.76
1:E:385:VAL:HG12	1:E:389:MET:HE2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:MET:HE1	1:C:383:ARG:HB2	1.67	0.75
1:E:385:VAL:CG1	1:E:389:MET:CE	2.62	0.74
1:C:33:CYS:SG	1:C:50:MET:HG2	2.28	0.73
2:L:158:ASN:HD21	2:L:189:ASP:H	1.37	0.73
1:C:95:HIS:HD2	1:C:128:THR:OG1	1.73	0.71
2:H:158:ASN:HD21	2:H:189:ASP:H	1.39	0.70
2:F:158:ASN:HD21	2:F:189:ASP:H	1.40	0.69
1:G:33:CYS:SG	1:G:50:MET:HG2	2.32	0.69
1:E:33:CYS:SG	1:E:50:MET:HG2	2.32	0.69
1:A:33:CYS:SG	1:A:50:MET:HG2	2.33	0.68
1:A:44:VAL:HG21	1:C:26:MET:HE3	1.73	0.68
1:A:26:MET:HE3	1:E:44:VAL:HG21	1.74	0.68
1:K:50[B]:MET:HE2	1:K:296:GLU:HB2	1.76	0.68
1:E:385:VAL:CG1	1:E:389:MET:HE2	2.21	0.68
1:K:223:LEU:C	1:K:223:LEU:HD23	2.19	0.67
1:A:26:MET:HE1	1:E:296:GLU:HG3	1.76	0.67
1:I:26:MET:HE1	1:K:296:GLU:HG3	1.77	0.66
1:I:131:GLU:HB3	1:I:155:ILE:HD11	1.78	0.65
1:E:131:GLU:HB3	1:E:155:ILE:HD11	1.79	0.64
1:C:131:GLU:HB3	1:C:155:ILE:HD11	1.78	0.64
1:G:131:GLU:HB3	1:G:155:ILE:HD11	1.79	0.64
1:A:131:GLU:HB3	1:A:155:ILE:HD11	1.79	0.63
1:K:131:GLU:HB3	1:K:155:ILE:HD11	1.80	0.63
1:A:151:ARG:NH1	4:A:501:HOH:O	2.30	0.62
2:D:219:LYS:NZ	4:D:301:HOH:O	2.30	0.62
1:A:296:GLU:HG3	1:C:26:MET:HE1	1.81	0.62
1:K:106:ARG:NH1	1:K:141:GLU:OE2	2.32	0.62
1:C:89:ASN:OD1	1:C:89:ASN:N	2.33	0.61
2:L:57:ASN:HD21	2:L:88:ASN:H	1.50	0.60
2:F:57:ASN:HD21	2:F:88:ASN:H	1.50	0.59
1:K:87:THR:HG23	1:K:89:ASN:OD1	2.03	0.59
2:J:28:LYS:O	2:J:28:LYS:HG3	2.02	0.59
2:L:51:LYS:HD2	2:L:53:LYS:HD3	1.84	0.58
1:G:84:LEU:HB3	1:G:92:MET:CE	2.33	0.58
1:C:131:GLU:CB	1:C:155:ILE:HD11	2.34	0.58
1:I:376:MET:HE3	1:I:383:ARG:HH12	1.63	0.58
2:F:28:LYS:O	2:F:28:LYS:HG3	2.03	0.58
2:J:57:ASN:HD21	2:J:88:ASN:H	1.51	0.58
1:K:84:LEU:HB3	1:K:92:MET:CE	2.32	0.58
2:H:57:ASN:HD21	2:H:88:ASN:H	1.52	0.58
1:G:284:THR:HG22	1:G:286:ALA:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:GLU:CB	1:E:155:ILE:HD11	2.34	0.57
1:I:131:GLU:CB	1:I:155:ILE:HD11	2.35	0.57
1:K:284:THR:HG22	1:K:286:ALA:H	1.70	0.56
2:H:28:LYS:O	2:H:28:LYS:HG3	2.04	0.56
2:L:28:LYS:O	2:L:28:LYS:HG3	2.05	0.56
1:K:113:ILE:HD12	1:K:199:ILE:CG2	2.35	0.56
1:C:80:THR:OG1	4:C:501:HOH:O	2.09	0.55
2:D:28:LYS:O	2:D:28:LYS:HG3	2.05	0.55
1:A:131:GLU:CB	1:A:155:ILE:HD11	2.35	0.55
1:G:131:GLU:CB	1:G:155:ILE:HD11	2.35	0.55
1:K:131:GLU:CB	1:K:155:ILE:HD11	2.36	0.55
1:I:26:MET:HE3	1:K:44:VAL:HG21	1.88	0.55
1:E:376:MET:HE1	1:E:383:ARG:CB	2.37	0.54
1:E:284:THR:HG22	1:E:286:ALA:H	1.71	0.54
1:I:376:MET:HE1	1:I:383:ARG:CB	2.36	0.54
1:I:42:GLY:HA3	3:I:501:EDO:H12	1.90	0.54
1:K:128:THR:OG1	1:K:207:LEU:HB3	2.07	0.54
1:K:388:GLN:OE1	4:K:501:HOH:O	2.18	0.53
1:C:128:THR:OG1	1:C:207:LEU:HB3	2.08	0.53
1:G:413:LEU:HG	1:G:415:LEU:CD1	2.39	0.53
1:G:129:PHE:CE2	1:G:163:ILE:HD13	2.44	0.53
1:A:376:MET:HE1	1:A:383:ARG:CB	2.38	0.52
1:C:80:THR:CG2	4:C:568:HOH:O	2.57	0.52
1:C:129:PHE:CE2	1:C:163:ILE:HD13	2.44	0.52
1:G:106:ARG:NH1	1:G:178:MET:HE2	2.25	0.52
1:C:376:MET:HE1	1:C:383:ARG:CB	2.38	0.51
1:I:56:LEU:O	1:I:354:THR:HG21	2.10	0.51
1:C:95:HIS:CD2	1:C:128:THR:OG1	2.61	0.51
1:A:360:SER:HB2	1:A:407:ILE:HD11	1.91	0.51
1:I:42:GLY:HA3	3:I:501:EDO:C1	2.41	0.51
1:G:335:GLY:H	2:H:141:ASN:HD22	1.57	0.51
1:C:176:ARG:HH12	1:C:196:LYS:HA	1.75	0.51
1:K:113:ILE:HD12	1:K:199:ILE:HG21	1.92	0.51
1:E:122:THR:HG23	1:E:198:THR:O	2.11	0.50
1:K:413:LEU:HG	1:K:415:LEU:CD1	2.42	0.50
1:C:80:THR:HG23	4:C:568:HOH:O	2.10	0.50
1:I:300:LYS:O	1:I:304:THR:HG23	2.11	0.49
1:C:124:ILE:CD1	1:C:199:ILE:HD11	2.43	0.48
2:B:214:LYS:O	2:B:218:LYS:HG3	2.13	0.48
1:C:306:ASN:ND2	4:C:506:HOH:O	2.45	0.48
1:K:81:VAL:HG12	1:K:83:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:214:LYS:O	2:L:218:LYS:HG3	2.14	0.48
1:A:59:ILE:HD11	1:A:371:LEU:HD21	1.95	0.48
2:B:219:LYS:O	2:B:220:LYS:HD2	2.14	0.48
1:K:284:THR:HG22	1:K:286:ALA:N	2.28	0.48
1:K:85:THR:N	1:K:92:MET:HE3	2.28	0.48
1:E:284:THR:HG22	1:E:286:ALA:N	2.29	0.47
1:I:91:SER:OG	1:I:125:GLU:HG2	2.13	0.47
1:K:33:CYS:SG	1:K:50[A]:MET:HG3	2.54	0.47
1:G:284:THR:HG22	1:G:286:ALA:N	2.30	0.47
2:D:53:LYS:HA	2:D:53:LYS:HD2	1.76	0.47
1:I:383:ARG:HH11	1:I:383:ARG:HG3	1.80	0.47
1:K:300:LYS:O	1:K:304:THR:HG23	2.15	0.47
1:G:85:THR:N	1:G:92:MET:HE3	2.31	0.46
1:C:128:THR:HG1	1:C:207:LEU:HB3	1.79	0.46
1:K:215:ASP:OD1	1:K:215:ASP:C	2.59	0.46
2:H:184:ILE:HG13	2:H:219:LYS:HD2	1.98	0.45
1:G:106:ARG:HH11	1:G:178:MET:HE2	1.81	0.45
1:E:128:THR:HA	1:E:205:SER:O	2.17	0.45
2:L:181:ASP:O	2:L:185:LYS:CG	2.65	0.45
1:E:144:ARG:NH1	4:E:509:HOH:O	2.49	0.45
1:I:368:PHE:C	1:I:368:PHE:CD1	2.95	0.45
1:I:300:LYS:O	1:I:304:THR:CG2	2.65	0.44
2:H:46:LYS:O	2:H:50:GLN:HG2	2.17	0.44
1:I:396:GLN:HG3	2:J:174:TYR:CE1	2.53	0.44
1:A:26:MET:CE	1:E:296:GLU:HG3	2.46	0.44
2:J:51:LYS:HE3	2:J:53:LYS:HG2	1.98	0.44
1:A:229:ARG:NH1	1:A:314:TYR:OH	2.50	0.44
1:C:195:GLU:OE2	4:C:502:HOH:O	2.21	0.44
1:G:210:ASN:HD22	1:G:210:ASN:HA	1.51	0.44
1:I:307:LYS:HD2	1:I:307:LYS:HA	1.85	0.44
1:G:128:THR:HA	1:G:205:SER:O	2.18	0.44
2:B:46:LYS:O	2:B:50:GLN:HG2	2.18	0.44
1:E:217:TYR:N	1:E:217:TYR:CD1	2.85	0.44
1:A:28:TYR:CD2	1:E:50:MET:HE1	2.53	0.43
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.84	0.43
1:A:128:THR:HA	1:A:205:SER:O	2.17	0.43
1:C:128:THR:HA	1:C:205:SER:O	2.18	0.43
1:E:137:TRP:CD2	1:E:169:SER:HB3	2.54	0.43
1:I:376:MET:CE	1:I:383:ARG:HH11	2.28	0.43
1:I:391:LYS:HZ1	2:J:107:ASP:CG	2.19	0.43
1:I:128:THR:HA	1:I:205:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:LYS:HD2	1:G:204:ILE:HD12	2.01	0.43
1:A:137:TRP:CD2	1:A:169:SER:HB3	2.53	0.43
1:E:84:LEU:HD13	1:E:119:MET:HE1	2.01	0.42
1:K:300:LYS:O	1:K:304:THR:CG2	2.67	0.42
1:G:413:LEU:HG	1:G:415:LEU:HD12	2.02	0.42
1:K:84:LEU:C	1:K:92:MET:HE3	2.45	0.42
1:G:368:PHE:CD1	1:G:368:PHE:C	2.97	0.42
1:C:79:LYS:HE3	4:C:564:HOH:O	2.18	0.42
1:G:385:VAL:HG21	3:I:501:EDO:H21	2.00	0.42
2:J:185:LYS:HB2	2:J:185:LYS:HE2	1.86	0.42
1:C:129:PHE:HE2	1:C:163:ILE:HD13	1.85	0.42
1:G:221:VAL:CG1	1:G:423:LEU:HB3	2.50	0.42
1:K:87:THR:CG2	1:K:89:ASN:OD1	2.66	0.42
1:I:59:ILE:HG23	1:I:354:THR:CG2	2.50	0.41
1:K:221:VAL:CG1	1:K:423:LEU:HB3	2.50	0.41
1:E:221:VAL:CG1	1:E:423:LEU:HB3	2.50	0.41
1:K:413:LEU:HG	1:K:415:LEU:HD12	2.03	0.41
1:E:27:VAL:HG11	1:E:389:MET:CE	2.51	0.41
1:G:84:LEU:C	1:G:92:MET:HE3	2.46	0.41
1:I:221:VAL:CG1	1:I:423:LEU:HB3	2.51	0.41
2:H:113:GLU:OE1	4:H:301:HOH:O	2.22	0.41
2:H:181:ASP:HB3	2:H:219:LYS:NZ	2.36	0.41
1:I:348:THR:CG2	1:I:383:ARG:NH1	2.84	0.41
1:K:128:THR:HA	1:K:205:SER:O	2.21	0.41
1:G:108:LEU:HD23	1:G:108:LEU:HA	1.85	0.41
2:L:171:VAL:HG11	2:L:179:ASP:HB3	2.03	0.41
2:J:201:LEU:HD21	2:J:205:LYS:HE3	2.02	0.40
1:K:87:THR:HG22	1:K:91:SER:O	2.21	0.40
1:G:137:TRP:CD2	1:G:169:SER:HB3	2.56	0.40
1:I:202:ARG:NH2	4:I:609:HOH:O	2.54	0.40
1:K:137:TRP:CD2	1:K:169:SER:HB3	2.56	0.40
1:E:408:GLN:HE22	1:G:409:TYR:H	1.70	0.40
1:G:307:LYS:HD2	1:G:307:LYS:HA	1.94	0.40
1:K:128:THR:OG1	1:K:129:PHE:N	2.53	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
2:D:220:LYS:NZ	2:J:162:THR:OG1[2_455]	2.08	0.12
1:E:151:ARG:NH2	1:I:202:ARG:NE[4_554]	2.17	0.03

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	399/401 (100%)	390 (98%)	9 (2%)	0	100	100
1	C	399/401 (100%)	388 (97%)	11 (3%)	0	100	100
1	E	399/401 (100%)	389 (98%)	10 (2%)	0	100	100
1	G	397/401 (99%)	389 (98%)	8 (2%)	0	100	100
1	I	399/401 (100%)	390 (98%)	9 (2%)	0	100	100
1	K	399/401 (100%)	390 (98%)	9 (2%)	0	100	100
2	B	191/193 (99%)	187 (98%)	4 (2%)	0	100	100
2	D	191/193 (99%)	189 (99%)	2 (1%)	0	100	100
2	F	191/193 (99%)	189 (99%)	2 (1%)	0	100	100
2	H	191/193 (99%)	188 (98%)	3 (2%)	0	100	100
2	J	191/193 (99%)	187 (98%)	4 (2%)	0	100	100
2	L	191/193 (99%)	187 (98%)	4 (2%)	0	100	100
All	All	3538/3564 (99%)	3463 (98%)	75 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	340/340 (100%)	323 (95%)	17 (5%)	22	41
1	C	340/340 (100%)	325 (96%)	15 (4%)	25	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	340/340 (100%)	325 (96%)	15 (4%)	25	47
1	G	339/340 (100%)	322 (95%)	17 (5%)	22	41
1	I	340/340 (100%)	320 (94%)	20 (6%)	18	34
1	K	341/340 (100%)	324 (95%)	17 (5%)	22	41
2	B	150/150 (100%)	149 (99%)	1 (1%)	76	88
2	D	150/150 (100%)	146 (97%)	4 (3%)	39	64
2	F	150/150 (100%)	146 (97%)	4 (3%)	39	64
2	H	150/150 (100%)	149 (99%)	1 (1%)	76	88
2	J	150/150 (100%)	145 (97%)	5 (3%)	33	58
2	L	150/150 (100%)	145 (97%)	5 (3%)	33	58
All	All	2940/2940 (100%)	2819 (96%)	121 (4%)	27	50

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	84	LEU
1	A	91	SER
1	A	108	LEU
1	A	122	THR
1	A	164	LYS
1	A	167	LYS
1	A	176	ARG
1	A	196	LYS
1	A	210	ASN
1	A	215	ASP
1	A	216	LYS
1	A	221	VAL
1	A	222	VAL
1	A	239	SER
1	A	372	LEU
1	A	393	LYS
2	B	190	LEU
1	C	80	THR
1	C	84	LEU
1	C	89	ASN
1	C	91	SER
1	C	128	THR

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Mol	Chain	Res	Type
1	C	163	ILE
1	C	164	LYS
1	C	210	ASN
1	C	217	TYR
1	C	222	VAL
1	C	239	SER
1	C	371	LEU
1	C	393	LYS
1	C	397	LEU
1	C	407	ILE
2	D	53	LYS
2	D	190	LEU
2	D	218	LYS
2	D	219	LYS
1	E	84	LEU
1	E	85	THR
1	E	91	SER
1	E	134	LEU
1	E	148	VAL
1	E	167	LYS
1	E	176	ARG
1	E	198	THR
1	E	221	VAL
1	E	239	SER
1	E	258	ASN
1	E	285	THR
1	E	371	LEU
1	E	393	LYS
1	E	407	ILE
2	F	154	LYS
2	F	171	VAL
2	F	190	LEU
2	F	219	LYS
1	G	84	LEU
1	G	91	SER
1	G	108	LEU
1	G	122	THR
1	G	163	ILE
1	G	164	LYS
1	G	176	ARG
1	G	190	LYS
1	G	198	THR

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Mol	Chain	Res	Type
1	G	210	ASN
1	G	216	LYS
1	G	221	VAL
1	G	239	SER
1	G	287	LYS
1	G	371	LEU
1	G	393	LYS
1	G	407	ILE
2	H	190	LEU
1	I	40	THR
1	I	84	LEU
1	I	123	LYS
1	I	134	LEU
1	I	167	LYS
1	I	176	ARG
1	I	178	MET
1	I	196	LYS
1	I	210	ASN
1	I	213	LYS
1	I	216	LYS
1	I	221	VAL
1	I	222	VAL
1	I	239	SER
1	I	304	THR
1	I	354	THR
1	I	371	LEU
1	I	383	ARG
1	I	393	LYS
1	I	407	ILE
2	J	53	LYS
2	J	86	LYS
2	J	154	LYS
2	J	190	LEU
2	J	218	LYS
1	K	40	THR
1	K	50[A]	MET
1	K	50[B]	MET
1	K	84	LEU
1	K	91	SER
1	K	128	THR
1	K	134	LEU
1	K	215	ASP

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Mol	Chain	Res	Type
1	K	216	LYS
1	K	221	VAL
1	K	239	SER
1	K	285	THR
1	K	304	THR
1	K	371	LEU
1	K	393	LYS
1	K	397	LEU
1	K	407	ILE
2	L	28	LYS
2	L	53	LYS
2	L	171	VAL
2	L	190	LEU
2	L	220	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	270	ASN
1	A	306	ASN
1	A	399	ASN
1	C	30	ASN
1	C	95	HIS
1	C	306	ASN
1	C	324	ASN
1	C	396	GLN
1	E	132	ASN
1	E	270	ASN
1	E	333	ASN
1	E	373	HIS
1	E	408	GLN
2	F	57	ASN
2	F	75	ASN
2	F	158	ASN
1	G	126	ASN
1	G	132	ASN
1	G	210	ASN
1	G	270	ASN
1	G	333	ASN
1	G	373	HIS
1	G	399	ASN

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Mol	Chain	Res	Type
2	H	57	ASN
2	H	75	ASN
2	H	141	ASN
2	H	158	ASN
1	I	126	ASN
1	I	132	ASN
1	I	270	ASN
1	I	333	ASN
1	I	373	HIS
1	I	388	GLN
1	I	392	ASN
2	J	57	ASN
2	J	59	GLN
2	J	140	GLN
1	K	30	ASN
1	K	132	ASN
1	K	203	ASN
1	K	270	ASN
1	K	306	ASN
1	K	333	ASN
1	K	373	HIS
2	L	57	ASN
2	L	75	ASN
2	L	158	ASN

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 ⓘ

1 ligand is 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	$\# Z > 2$
3	EDO	I	501	-	3,3,3	1.11	0	2,2,2	0.84	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	EDO	I	501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	501	EDO	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	401/401 (100%)	0.26	19 (4%) 36 32	17, 31, 66, 143	0
1	C	401/401 (100%)	0.84	69 (17%) 4 3	15, 36, 99, 146	0
1	E	401/401 (100%)	0.54	26 (6%) 25 22	17, 37, 74, 128	0
1	G	399/401 (99%)	0.88	55 (13%) 6 5	17, 42, 95, 224	0
1	I	401/401 (100%)	0.55	35 (8%) 16 14	10, 34, 79, 181	0
1	K	400/401 (99%)	0.50	36 (9%) 15 13	14, 35, 85, 129	1 (0%)
2	B	193/193 (100%)	0.27	10 (5%) 33 29	24, 38, 72, 141	0
2	D	193/193 (100%)	0.28	9 (4%) 36 32	24, 37, 68, 100	0
2	F	193/193 (100%)	0.46	14 (7%) 21 18	28, 43, 83, 120	0
2	H	193/193 (100%)	0.43	10 (5%) 33 29	27, 40, 68, 111	0
2	J	193/193 (100%)	0.56	19 (9%) 13 11	26, 47, 82, 118	0
2	L	193/193 (100%)	0.31	11 (5%) 29 26	23, 40, 82, 131	0
All	All	3561/3564 (99%)	0.53	313 (8%) 15 13	10, 38, 84, 224	1 (0%)

All (313) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	380	SER	10.0
1	I	384	GLY	9.6
1	I	385	VAL	9.0
1	I	383	ARG	8.3
1	I	386	ALA	8.2
1	I	387	SER	8.2
1	G	383	ARG	7.6
1	G	379	SER	7.5
1	E	382	ASP	7.2
1	G	385	VAL	7.2
1	C	380	SER	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	385	VAL	7.1
1	I	390	ILE	6.9
1	G	381	SER	6.9
1	G	377	ASP	6.8
1	I	389	MET	6.8
1	G	376	MET	6.5
1	A	382	ASP	6.5
1	A	386	ALA	6.2
1	G	378	GLN	6.1
1	E	385	VAL	6.0
1	E	383	ARG	6.0
1	G	382	ASP	5.9
1	C	376	MET	5.8
1	A	383	ARG	5.6
2	L	215	ALA	5.5
1	I	396	GLN	5.5
1	E	390	ILE	5.5
1	A	387	SER	5.4
1	C	377	ASP	5.4
1	I	388	GLN	5.3
1	E	387	SER	5.3
1	E	386	ALA	5.3
1	G	386	ALA	5.3
1	A	384	GLY	5.2
1	G	384	GLY	5.2
1	I	392	ASN	5.1
1	C	181	LYS	5.1
1	I	394	ILE	5.1
1	I	397	LEU	5.0
1	G	387	SER	5.0
1	I	398	ILE	4.9
1	C	187	THR	4.9
1	I	400	LYS	4.9
1	C	197	PRO	4.8
1	G	88	ALA	4.8
1	C	196	LYS	4.8
2	B	220	LYS	4.8
1	C	182	LEU	4.7
1	C	184	GLU	4.7
1	I	393	LYS	4.7
1	I	401	ARG	4.6
2	L	219	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	G	390	ILE	4.6
1	K	146	GLY	4.5
1	C	193	MET	4.4
1	C	194	LEU	4.4
1	C	179	TYR	4.4
1	C	186	ALA	4.3
1	C	188	LYS	4.3
1	I	88	ALA	4.3
1	C	192	PHE	4.2
2	L	216	LEU	4.2
1	E	389	MET	4.2
1	C	190	LYS	4.2
1	E	384	GLY	4.2
2	F	220	LYS	4.2
1	I	391	LYS	4.2
1	G	210	ASN	4.1
1	C	374	THR	4.1
2	J	220	LYS	4.1
2	L	220	LYS	4.0
2	F	219	LYS	4.0
1	C	154	THR	4.0
1	A	388	GLN	4.0
1	E	388	GLN	4.0
1	K	88	ALA	3.9
1	C	155	ILE	3.9
1	C	180	SER	3.9
1	C	189	ALA	3.9
1	C	383	ARG	3.9
1	C	375	ASP	3.8
1	C	185	ARG	3.8
1	A	390	ILE	3.8
1	K	192	PHE	3.8
1	C	385	VAL	3.7
1	A	389	MET	3.7
2	L	217	SER	3.7
1	C	195	GLU	3.7
1	C	216	LYS	3.7
1	C	373	HIS	3.7
1	G	213	LYS	3.7
1	C	183	ARG	3.7
1	K	145	ILE	3.6
1	I	89	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	198	THR	3.6
2	D	217	SER	3.6
1	C	379	SER	3.6
1	C	191	VAL	3.6
1	E	393	LYS	3.6
1	K	117	ASN	3.5
1	G	389	MET	3.5
1	C	381	SER	3.5
1	G	208	PRO	3.5
2	B	53	LYS	3.5
2	D	220	LYS	3.5
2	F	28	LYS	3.5
2	J	219	LYS	3.5
1	K	128	THR	3.4
1	A	393	LYS	3.4
1	K	148	VAL	3.4
1	C	210	ASN	3.4
1	I	399	ASN	3.4
1	G	211	ASN	3.4
1	K	127	LEU	3.3
1	C	213	LYS	3.3
2	D	218	LYS	3.3
2	B	49	VAL	3.3
1	K	187	THR	3.3
2	J	28	LYS	3.3
1	C	378	GLN	3.3
1	I	90	GLY	3.3
1	C	164	LYS	3.3
2	F	215	ALA	3.2
2	H	220	LYS	3.2
2	D	86	LYS	3.1
1	A	146	GLY	3.1
2	L	51	LYS	3.1
1	C	387	SER	3.1
1	K	199	ILE	3.1
1	G	388	GLN	3.1
2	B	52	ASN	3.1
2	D	50	GLN	3.1
2	B	219	LYS	3.1
1	C	384	GLY	3.1
2	H	49	VAL	3.1
2	B	51	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	382	ASP	3.0
2	F	211	ASP	3.0
2	J	53	LYS	3.0
1	A	148	VAL	3.0
1	E	341	SER	3.0
2	H	219	LYS	3.0
1	I	332	ASP	3.0
2	D	52	ASN	3.0
1	C	88	ALA	2.9
1	I	395	SER	2.9
2	J	86	LYS	2.9
1	K	84	LEU	2.9
1	G	215	ASP	2.9
1	I	324	ASN	2.9
1	A	397	LEU	2.9
1	G	393	LYS	2.8
1	G	207	LEU	2.8
1	K	71	LYS	2.8
1	G	126	ASN	2.8
2	L	218	LYS	2.8
1	G	174	ILE	2.8
1	C	86	PRO	2.8
1	G	116	LEU	2.8
2	F	143	LYS	2.8
1	K	91	SER	2.7
1	K	120	LYS	2.7
2	F	210	GLN	2.7
1	C	178	MET	2.7
2	J	215	ALA	2.7
1	G	204	ILE	2.7
1	E	392	ASN	2.7
2	L	28	LYS	2.7
1	C	152	TYR	2.7
2	J	51	LYS	2.6
1	C	371	LEU	2.6
1	C	372	LEU	2.6
1	K	217	TYR	2.6
1	K	424	THR	2.6
1	E	216	LYS	2.6
2	H	53	LYS	2.6
1	A	401	ARG	2.6
1	G	131	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	159	ALA	2.6
1	C	161	ALA	2.6
1	E	218	THR	2.6
1	I	425	GLU	2.6
1	E	394	ILE	2.5
1	A	211	ASN	2.5
2	B	50	GLN	2.5
2	J	84	SER	2.5
1	C	217	TYR	2.5
1	C	90	GLY	2.5
1	K	147	GLY	2.5
1	A	394	ILE	2.5
1	G	192	PHE	2.5
1	K	111	PHE	2.5
2	B	218	LYS	2.5
2	J	213	ALA	2.5
1	E	335	GLY	2.5
1	C	156	GLU	2.5
1	G	200	GLU	2.5
1	C	170	PHE	2.5
1	K	126	ASN	2.5
1	C	173	ALA	2.5
1	G	154	THR	2.5
1	G	199	ILE	2.5
1	I	181	LYS	2.5
2	J	50	GLN	2.5
1	A	392	ASN	2.5
1	E	176	ARG	2.5
1	E	255	ALA	2.5
1	G	212	TYR	2.4
2	J	218	LYS	2.4
2	H	50	GLN	2.4
1	G	132	ASN	2.4
1	C	153	GLU	2.4
2	L	50	GLN	2.4
1	G	129	PHE	2.4
1	C	386	ALA	2.4
1	G	172	THR	2.4
2	J	117	LYS	2.4
2	F	50	GLN	2.4
1	G	148	VAL	2.4
1	G	177	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	145	THR	2.4
1	C	169	SER	2.4
1	G	194	LEU	2.4
1	G	217	TYR	2.4
2	J	52	ASN	2.4
1	K	216	LYS	2.4
1	C	151	ARG	2.3
1	C	129	PHE	2.3
1	I	217	TYR	2.3
2	J	214	LYS	2.3
2	J	151	ALA	2.3
1	I	408	GLN	2.3
1	C	134	LEU	2.3
2	J	216	LEU	2.3
2	B	28	LYS	2.3
1	C	148	VAL	2.3
1	G	203	ASN	2.3
1	K	94	LEU	2.3
1	K	413	LEU	2.3
2	H	216	LEU	2.3
1	E	215	ASP	2.3
1	G	216	LYS	2.3
1	C	80	THR	2.3
1	G	109	SER	2.3
1	K	421	SER	2.3
2	J	217	SER	2.3
1	G	127	LEU	2.3
1	C	203	ASN	2.2
1	K	118	ARG	2.3
1	E	397	LEU	2.2
2	L	48	LEU	2.2
1	K	417	PHE	2.2
1	K	221	VAL	2.2
2	F	49	VAL	2.2
1	C	128	THR	2.2
1	G	119	MET	2.2
1	K	209	LYS	2.2
2	F	216	LEU	2.2
2	L	54	ILE	2.2
2	H	110	ASP	2.2
1	I	170	PHE	2.2
2	J	49	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	181	LYS	2.2
1	G	214	LYS	2.2
1	K	212	TYR	2.2
1	C	145	ILE	2.2
1	K	215	ASP	2.2
1	G	391	LYS	2.2
2	H	52	ASN	2.2
1	A	154	THR	2.2
1	G	94	LEU	2.2
1	E	153	GLU	2.2
1	K	425	GLU	2.2
1	G	170	PHE	2.2
2	F	151	ALA	2.1
1	C	423	LEU	2.1
1	E	182	LEU	2.1
1	G	113	ILE	2.1
1	I	199	ILE	2.1
2	J	54	ILE	2.1
1	C	160	GLU	2.1
1	I	176	ARG	2.1
1	I	202	ARG	2.1
2	D	49	VAL	2.1
1	K	189	ALA	2.1
1	A	398	ILE	2.1
1	I	155	ILE	2.1
1	G	209	LYS	2.1
2	F	53	LYS	2.1
2	H	51	LYS	2.1
1	C	158	GLN	2.1
1	E	408	GLN	2.1
1	G	221	VAL	2.1
1	G	198	THR	2.1
1	E	401	ARG	2.1
1	I	188	LYS	2.1
1	K	180	SER	2.1
1	G	222	VAL	2.1
1	E	214	LYS	2.1
2	D	51	LYS	2.1
2	F	218	LYS	2.1
1	C	143	PRO	2.1
1	K	123	LYS	2.0
1	K	201	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	94	LEU	2.0
1	G	159	ALA	2.0
1	K	214	LYS	2.0
2	D	219	LYS	2.0
2	H	214	LYS	2.0
1	I	124	ILE	2.0
2	B	54	ILE	2.0
1	K	142	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	I	501	4/4	0.79	0.21	31,37,37,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.