Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:16 PM GMT

PDB ID	:	5CER
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

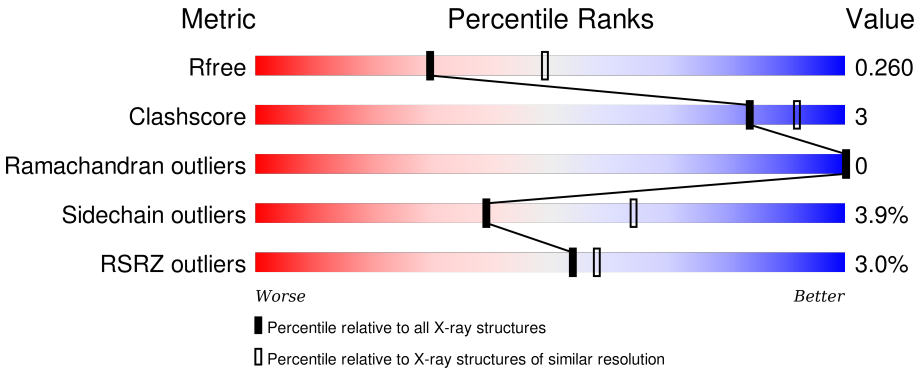
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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}	91344	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	2% 90% 9%
1	C	401	5% 90% 7%
1	E	401	% 88% 11%
1	G	401	5% 89% 10%
1	I	401	3% 90% 9%

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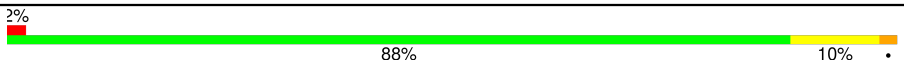
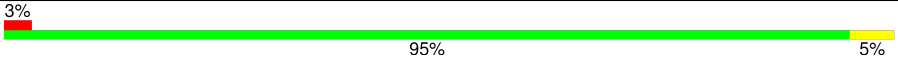
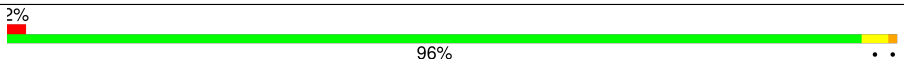
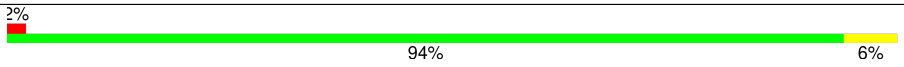
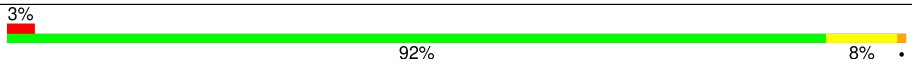
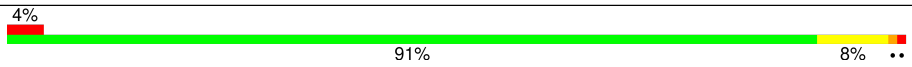
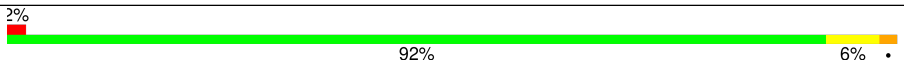
Mol	Chain	Length	Quality of chain
1	K	401	
2	B	193	
2	D	193	
2	F	193	
2	H	193	
2	J	193	
2	L	193	

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			

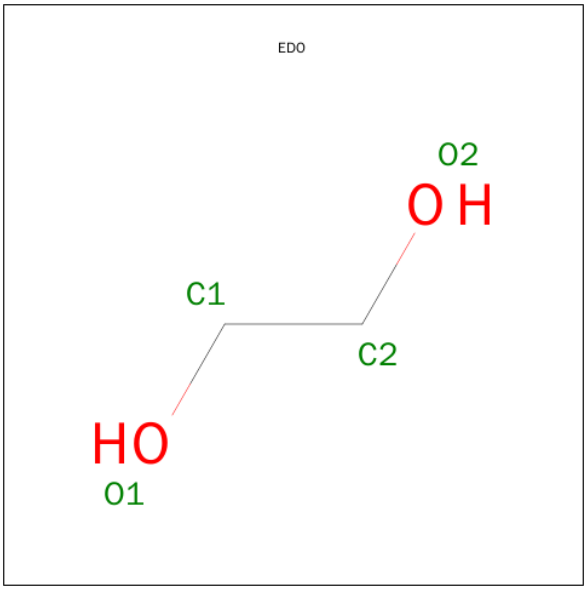
There are 12 discrepancies between the modelled and reference sequences:

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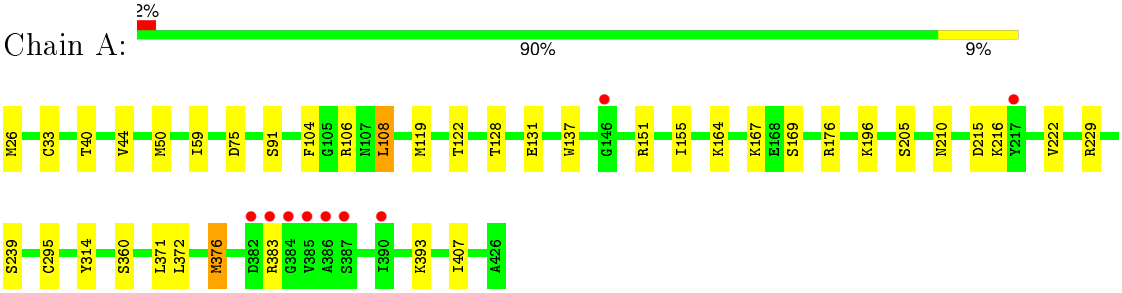
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	94	Total O 94 94	0	0
4	E	141	Total O 141 141	0	0
4	F	77	Total O 77 77	0	0
4	G	112	Total O 112 112	0	0
4	H	84	Total O 84 84	0	0
4	I	131	Total O 131 131	0	0
4	J	69	Total O 69 69	0	0
4	K	136	Total O 136 136	0	0
4	L	97	Total O 97 97	0	0

3 Residue-property plots (i)

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.

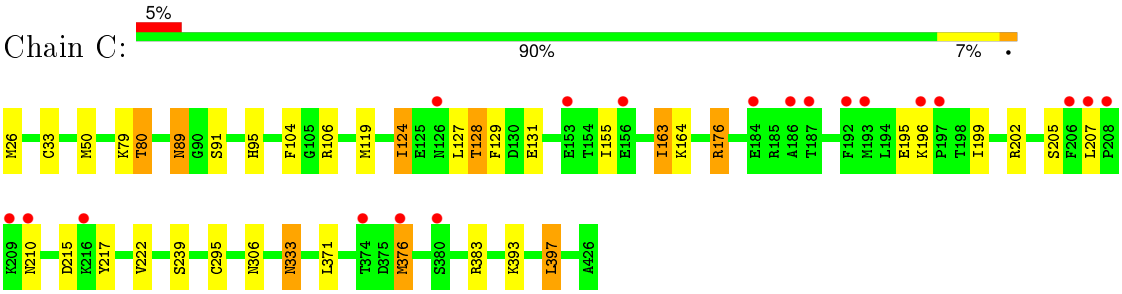
- Molecule 1: Bd0816

Chain A:



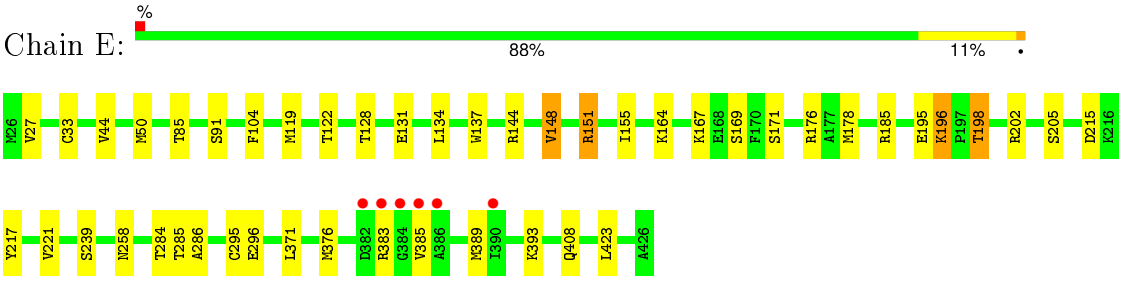
- Molecule 1: Bd0816

Chain C:



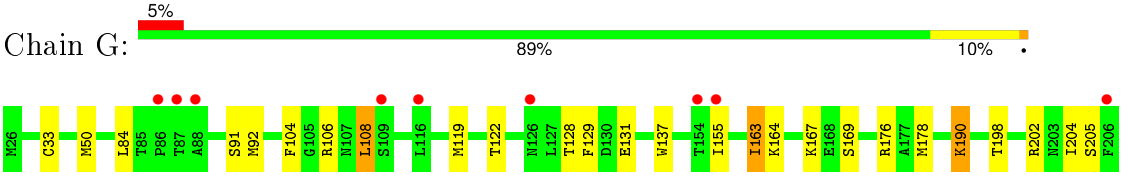
- Molecule 1: Bd0816

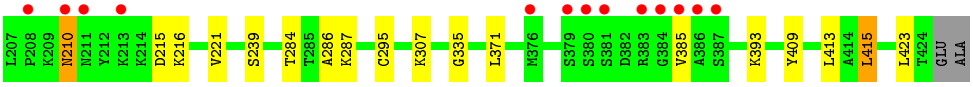
Chain E:



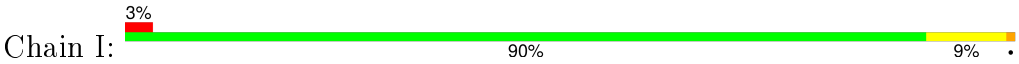
- Molecule 1: Bd0816

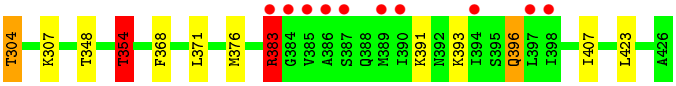
Chain G:



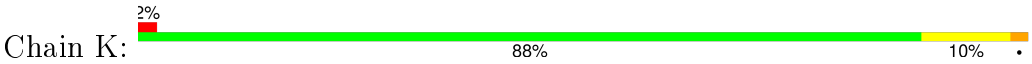


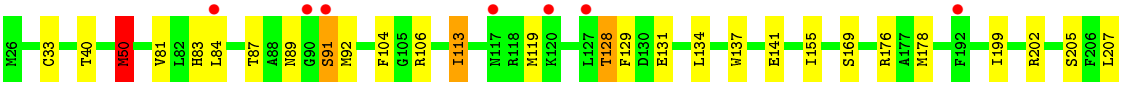
• Molecule 1: Bd0816

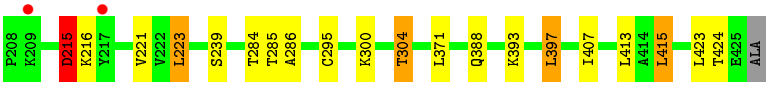




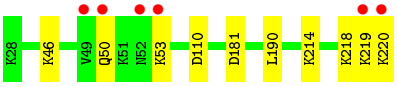
• Molecule 1: Bd0816



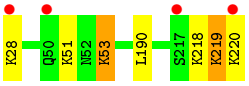




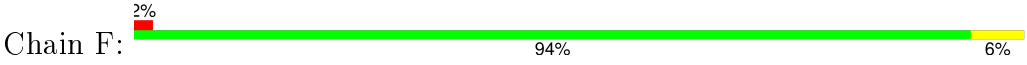
• Molecule 2: Bd3460

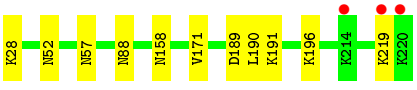


• Molecule 2: Bd3460

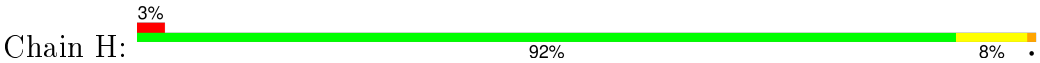


• Molecule 2: Bd3460



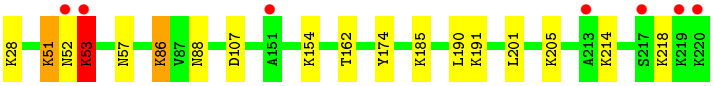


• Molecule 2: Bd3460



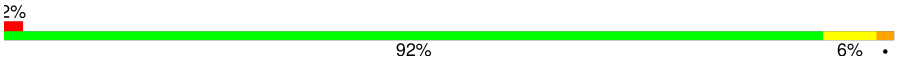
- Molecule 2: Bd3460

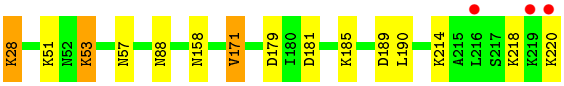
Chain J:



- Molecule 2: Bd3460

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 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 – 2.48 103.62 – 2.48	Depositor EDS
% Data completeness (in resolution range)	98.8 (100.00-2.48) 98.8 (103.62-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	3.73 (at 2.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.249 0.233 , 0.260	Depositor DCC
R_{free} test set	7978 reflections (5.21%)	DCC
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 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 161147 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.71	0/3176	0.84	5/4287 (0.1%)
1	C	0.72	1/3176 (0.0%)	0.88	8/4287 (0.2%)
1	E	0.73	1/3176 (0.0%)	0.89	12/4287 (0.3%)
1	G	0.64	0/3162	0.86	10/4268 (0.2%)
1	I	0.73	1/3176 (0.0%)	0.86	7/4287 (0.2%)
1	K	0.69	0/3179	0.89	10/4290 (0.2%)
2	B	0.69	1/1447 (0.1%)	0.77	2/1940 (0.1%)
2	D	0.63	0/1447	0.79	1/1940 (0.1%)
2	F	0.61	0/1447	0.78	2/1940 (0.1%)
2	H	0.63	0/1447	0.78	3/1940 (0.2%)
2	J	0.63	0/1447	0.83	4/1940 (0.2%)
2	L	0.65	0/1447	0.79	0/1940
All	All	0.68	4/27727 (0.0%)	0.85	64/37346 (0.2%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	171	SER	CA-CB	7.87	1.64	1.52
1	I	91	SER	CB-OG	-6.99	1.33	1.42
1	C	333	ASN	C-N	6.23	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	53	LYS	CD-CE	5.11	1.64	1.51

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	223	LEU	CB-CG-CD2	-11.33	91.74	111.00
1	E	185	ARG	CG-CD-NE	9.56	131.89	111.80
1	C	124	ILE	CG1-CB-CG2	-9.48	90.53	111.40
1	I	383	ARG	CG-CD-NE	8.72	130.11	111.80
1	E	178	MET	CG-SD-CE	8.59	113.94	100.20
1	G	215	ASP	CB-CG-OD1	7.73	125.25	118.30
1	K	415	LEU	CB-CG-CD2	7.51	123.76	111.00
1	G	415	LEU	CB-CG-CD2	7.38	123.55	111.00
1	K	113	ILE	CA-CB-CG1	7.29	124.85	111.00
1	G	202	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	K	178	MET	CG-SD-CE	7.18	111.69	100.20
1	G	163	ILE	CA-CB-CG1	7.07	124.42	111.00
2	J	86	LYS	CA-CB-CG	7.01	128.81	113.40
1	G	178	MET	CG-SD-CE	6.95	111.32	100.20
1	C	163	ILE	CA-CB-CG1	6.92	124.16	111.00
1	K	397	LEU	CA-CB-CG	6.85	131.06	115.30
1	G	106	ARG	NE-CZ-NH2	-6.69	116.96	120.30
2	D	51	LYS	CB-CA-C	-6.66	97.08	110.40
2	J	51	LYS	CB-CA-C	-6.60	97.19	110.40
1	E	215	ASP	CB-CG-OD2	6.44	124.10	118.30
1	A	372	LEU	CA-CB-CG	6.42	130.06	115.30
1	C	397	LEU	CA-CB-CG	6.35	129.91	115.30
1	I	106	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	I	106	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	I	215	ASP	CB-CG-OD1	6.08	123.78	118.30
1	G	190	LYS	CA-CB-CG	6.08	126.78	113.40
2	F	191	LYS	CD-CE-NZ	5.97	125.44	111.70
1	I	396	GLN	CA-CB-CG	5.97	126.53	113.40
1	K	50[A]	MET	CA-CB-CG	5.93	123.38	113.30
1	K	50[B]	MET	CA-CB-CG	5.93	123.38	113.30
2	J	191	LYS	CD-CE-NZ	5.87	125.21	111.70
1	G	106	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	E	202	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	119	MET	CA-CB-CG	5.77	123.11	113.30
1	E	195	GLU	C-N-CA	5.69	135.93	121.70
1	E	196	LYS	CB-CA-C	-5.68	99.05	110.40
2	J	53	LYS	CB-CA-C	5.60	121.59	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	202	ARG	CA-CB-CG	5.57	125.65	113.40
1	C	202	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	E	185	ARG	CD-NE-CZ	-5.55	115.83	123.60
1	I	354	THR	N-CA-CB	-5.54	99.78	110.30
1	C	119	MET	CA-CB-CG	5.52	122.68	113.30
1	G	106	ARG	CG-CD-NE	-5.51	100.23	111.80
1	E	119	MET	CA-CB-CG	5.45	122.56	113.30
1	E	148	VAL	CB-CA-C	5.43	121.72	111.40
1	C	376	MET	CG-SD-CE	-5.37	91.60	100.20
1	K	215	ASP	CB-CA-C	5.37	121.13	110.40
2	H	219	LYS	CD-CE-NZ	5.33	123.95	111.70
1	A	106	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	376	MET	CG-SD-CE	-5.29	91.73	100.20
2	F	196	LYS	CD-CE-NZ	5.29	123.86	111.70
2	H	110	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	K	119	MET	CA-CB-CG	5.27	122.26	113.30
1	G	119	MET	CA-CB-CG	5.26	122.24	113.30
2	B	110	ASP	CB-CG-OD1	5.21	122.99	118.30
1	E	164	LYS	CD-CE-NZ	5.21	123.69	111.70
1	E	151	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	I	215	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	E	196	LYS	N-CA-CB	-5.14	101.34	110.60
2	H	196	LYS	CG-CD-CE	5.13	127.29	111.90
2	B	181	ASP	CB-CA-C	-5.13	100.15	110.40
1	C	106	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	127	LEU	CB-CG-CD1	5.06	119.60	111.00
1	A	372	LEU	CB-CG-CD2	-5.04	102.44	111.00

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 (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3124	0	3148	18	0
1	C	3124	0	3148	24	0
1	E	3124	0	3148	25	1
1	G	3110	0	3137	23	0
1	I	3124	0	3148	25	1
1	K	3124	0	3152	29	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	1.83	0.94
1:A:75:ASP:OD1	1:A:229:ARG:NH1	2.08	0.85
1:E:385:VAL:HG12	1:E:389:MET:HE2	1.57	0.85
1:I:376:MET:CE	1:I:383:ARG:NH1	2.46	0.78
1:E:385:VAL:HG12	1:E:389:MET:HE3	1.64	0.77
1:E:385:VAL:CG1	1:E:389:MET:HE2	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:K:223:LEU:HD23	1:K:223:LEU:C	2.19	0.62
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: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:I:376:MET:HE3	1:I:383:ARG:HH11	1.65	0.59
1:K:87:THR:HG23	1:K:89:ASN:OD1	2.03	0.59
2:J:28:LYS:HG3	2:J:28:LYS:O	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:K:84:LEU:HB3	1:K:92:MET:CE	2.32	0.58
1:C:131:GLU:CB	1:C:155:ILE:HD11	2.34	0.58
2:J:57:ASN:HD21	2:J:88:ASN:H	1.51	0.58
2:F:28:LYS:HG3	2:F:28:LYS:O	2.03	0.58
2:H:57:ASN:HD21	2:H:88:ASN:H	1.52	0.58
2:H:28:LYS:HG3	2:H:28:LYS:O	2.04	0.58
1:G:284:THR:HG22	1:G:286:ALA:H	1.69	0.58
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:A:376:MET:HE3	1:A:383:ARG:HE	1.70	0.57
1:K:284:THR:HG22	1:K:286:ALA:H	1.70	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:A:44:VAL:HG21	1:C:26:MET:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:THR:OG1	4:C:501:HOH:O	2.09	0.55
2:D:28:LYS:HG3	2:D:28:LYS:O	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:C:376:MET:HE3	1:C:383:ARG:HE	1.72	0.55
1:E:284:THR:HG22	1:E:286:ALA:H	1.71	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:84:LEU:HB3	1:K:92:MET:HE2	1.88	0.54
1:E:27:VAL:HG11	1:E:389:MET:HE3	1.88	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:E:376:MET:HE3	1:E:383:ARG:HE	1.73	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: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:I:33:CYS:HG	1:I:295:CYS:HB3	1.75	0.51
1:A:26:MET:HE3	1:E:44:VAL:HG21	1.92	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:33:CYS:HG	1:A:295:CYS:HB3	1.74	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:K:33:CYS:HG	1:K:295:CYS:HB3	1.76	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:33:CYS:HG	1:E:295:CYS:HB3	1.77	0.50
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:G:84:LEU:HB3	1:G:92:MET:HE2	1.93	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:284:THR:HG22	1:K:286:ALA:N	2.28	0.48
2:B:219:LYS:O	2:B:220:LYS:HD2	2.14	0.48
1:E:284:THR:HG22	1:E:286:ALA:N	2.29	0.47
1:K:33:CYS:SG	1:K:50[A]:MET:HG3	2.54	0.47
1:I:91:SER:OG	1:I:125:GLU:HG2	2.13	0.47
1:G:284:THR:HG22	1:G:286:ALA:N	2.30	0.47
2:D:53:LYS:HD2	2:D:53:LYS:HA	1.76	0.47
1:I:383:ARG:HG3	1:I:383:ARG:HH11	1.80	0.47
1:C:33:CYS:HG	1:C:295:CYS:HB3	1.80	0.47
1:K:300:LYS:O	1:K:304:THR:HG23	2.15	0.47
1:A:33:CYS:HG	1:A:295:CYS:CB	2.27	0.47
1:C:128:THR:HG1	1:C:207:LEU:HB3	1.79	0.46
1:G:84:LEU:HB3	1:G:92:MET:HE3	1.96	0.46
1:A:26:MET:CE	1:E:296:GLU:HG3	2.46	0.46
1:K:33:CYS:HG	1:K:295:CYS:CB	2.28	0.46
1:I:33:CYS:HG	1:I:295:CYS:CB	2.29	0.46
2:H:184:ILE:HG13	2:H:219:LYS:HD2	1.98	0.45
1:E:128:THR:HA	1:E:205:SER:O	2.17	0.45
1:E:33:CYS:HG	1:E:295:CYS:CB	2.30	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:300:LYS:O	1:I:304:THR:CG2	2.65	0.44
1:G:33:CYS:HG	1:G:295:CYS:HB3	1.81	0.44
1:I:391:LYS:NZ	2:J:107:ASP:OD2	2.37	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
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:HA	1:I:307:LYS:HD2	1.85	0.44
1:G:128:THR:HA	1:G:205:SER:O	2.18	0.44
1:E:217:TYR:N	1:E:217:TYR:CD1	2.85	0.44
2:B:46:LYS:O	2:B:50:GLN:HG2	2.18	0.44
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:I:376:MET:CE	1:I:383:ARG:HB2	2.48	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:128:THR:HA	1:I:205:SER:O	2.18	0.43
1:I:376:MET:HE3	1:I:383:ARG:HB2	2.00	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:A:376:MET:CE	1:A:383:ARG:HB2	2.50	0.42
1:K:300:LYS:O	1:K:304:THR:CG2	2.67	0.42
1:K:84:LEU:HB3	1:K:92:MET:HE3	2.00	0.42
1:G:413:LEU:HG	1:G:415:LEU:HD12	2.02	0.42
1:E:376:MET:CE	1:E:383:ARG:HB2	2.49	0.42
1:C:33:CYS:HG	1:C:295:CYS:CB	2.31	0.42
1:G:33:CYS:HG	1:G:295:CYS:CB	2.33	0.42
1:G:385:VAL:HG21	3:I:501:EDO:H21	2.00	0.42
1:C:79:LYS:HE3	4:C:564:HOH:O	2.18	0.42
2:J:185:LYS:HE2	2:J:185:LYS:HB2	1.86	0.42
1:K:87:THR:CG2	1:K:89:ASN:OD1	2.66	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:C:376:MET:CE	1:C:383:ARG:HB2	2.50	0.41
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:K:413:LEU:HG	1:K:415:LEU:HD12	2.03	0.41
1:E:221:VAL:CG1	1:E:423:LEU:HB3	2.50	0.41
1:E:27:VAL:HG11	1:E:389:MET:CE	2.51	0.41
1:K:215:ASP:OD1	1:K:215:ASP:C	2.59	0.41
1:I:221:VAL:CG1	1:I:423:LEU:HB3	2.51	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
2:H:181:ASP:HB3	2:H:219:LYS:NZ	2.36	0.41
2:H:113:GLU:OE1	4:H:301:HOH:O	2.22	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
1:K:87:THR:HG22	1:K:91:SER:O	2.21	0.40
2:J:201:LEU:HD21	2:J:205:LYS:HE3	2.02	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:K:128:THR:OG1	1:K:129:PHE:N	2.53	0.40
1:I:368:PHE:CD1	1:I:368:PHE:C	2.95	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

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 (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	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 (i)

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%)	325 (96%)	15 (4%)	35	58
1	C	340/340 (100%)	325 (96%)	15 (4%)	35	58
1	E	340/340 (100%)	327 (96%)	13 (4%)	40	65
1	G	339/340 (100%)	325 (96%)	14 (4%)	37	62
1	I	340/340 (100%)	322 (95%)	18 (5%)	28	48
1	K	341/340 (100%)	324 (95%)	17 (5%)	30	52
2	B	150/150 (100%)	149 (99%)	1 (1%)	88	96
2	D	150/150 (100%)	146 (97%)	4 (3%)	52	78
2	F	150/150 (100%)	146 (97%)	4 (3%)	52	78
2	H	150/150 (100%)	148 (99%)	2 (1%)	76	91
2	J	150/150 (100%)	143 (95%)	7 (5%)	32	55
2	L	150/150 (100%)	145 (97%)	5 (3%)	45	71
All	All	2940/2940 (100%)	2825 (96%)	115 (4%)	39	64

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	91	SER
1	A	104	PHE
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	222	VAL
1	A	239	SER
1	A	393	LYS
2	B	190	LEU
1	C	80	THR
1	C	89	ASN
1	C	91	SER
1	C	104	PHE

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Mol	Chain	Res	Type
1	C	128	THR
1	C	164	LYS
1	C	176	ARG
1	C	210	ASN
1	C	215	ASP
1	C	217	TYR
1	C	222	VAL
1	C	239	SER
1	C	371	LEU
1	C	393	LYS
1	C	397	LEU
2	D	53	LYS
2	D	190	LEU
2	D	218	LYS
2	D	219	LYS
1	E	85	THR
1	E	91	SER
1	E	104	PHE
1	E	134	LEU
1	E	148	VAL
1	E	167	LYS
1	E	176	ARG
1	E	198	THR
1	E	239	SER
1	E	258	ASN
1	E	285	THR
1	E	371	LEU
1	E	393	LYS
2	F	52	ASN
2	F	171	VAL
2	F	190	LEU
2	F	219	LYS
1	G	91	SER
1	G	104	PHE
1	G	108	LEU
1	G	122	THR
1	G	164	LYS
1	G	176	ARG
1	G	190	LYS
1	G	198	THR
1	G	210	ASN
1	G	216	LYS

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Mol	Chain	Res	Type
1	G	239	SER
1	G	287	LYS
1	G	371	LEU
1	G	393	LYS
2	H	52	ASN
2	H	190	LEU
1	I	40	THR
1	I	104	PHE
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	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	52	ASN
2	J	53	LYS
2	J	86	LYS
2	J	154	LYS
2	J	190	LEU
2	J	214	LYS
2	J	218	LYS
1	K	40	THR
1	K	50[A]	MET
1	K	50[B]	MET
1	K	91	SER
1	K	104	PHE
1	K	128	THR
1	K	134	LEU
1	K	176	ARG
1	K	215	ASP
1	K	216	LYS
1	K	239	SER

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Mol	Chain	Res	Type
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

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

Mol	Chain	Res	Type
1	A	126	ASN
1	A	210	ASN
2	B	210	GLN
1	C	30	ASN
1	C	95	HIS
1	C	306	ASN
1	E	132	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	333	ASN
1	G	373	HIS
2	H	57	ASN
2	H	59	GLN
2	H	75	ASN
2	H	141	ASN
2	H	158	ASN
2	H	210	GLN
1	I	126	ASN
1	I	132	ASN
1	I	236	ASN

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Mol	Chain	Res	Type
1	I	333	ASN
1	I	373	HIS
2	J	57	ASN
2	J	59	GLN
2	J	106	ASN
2	J	141	ASN
1	K	30	ASN
1	K	132	ASN
1	K	236	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 carbohydrates 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	1.10	0	2,2,2	0.96	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	0/0/0/0

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, 95^{th} 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%)	-0.16	9 (2%) 65 69	17, 31, 66, 143	0
1	C	401/401 (100%)	0.13	19 (4%) 35 39	15, 36, 99, 146	0
1	E	401/401 (100%)	-0.01	6 (1%) 76 79	17, 37, 74, 128	0
1	G	399/401 (99%)	0.21	22 (5%) 29 32	17, 42, 95, 224	0
1	I	401/401 (100%)	-0.04	14 (3%) 48 52	10, 34, 79, 181	0
1	K	400/401 (99%)	-0.03	9 (2%) 64 67	14, 35, 85, 129	0
2	B	193/193 (100%)	-0.04	6 (3%) 52 56	24, 38, 72, 141	0
2	D	193/193 (100%)	-0.20	4 (2%) 67 70	24, 37, 68, 100	0
2	F	193/193 (100%)	-0.09	3 (1%) 74 77	28, 43, 83, 120	0
2	H	193/193 (100%)	-0.03	5 (2%) 59 63	27, 40, 68, 111	0
2	J	193/193 (100%)	0.06	7 (3%) 46 51	26, 47, 82, 118	0
2	L	193/193 (100%)	-0.19	3 (1%) 74 77	23, 40, 82, 131	0
All	All	3561/3564 (99%)	-0.01	107 (3%) 54 58	10, 38, 84, 224	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	220	LYS	15.3
2	F	220	LYS	7.4
1	G	210	ASN	5.7
2	B	52	ASN	5.5
2	J	220	LYS	5.4
2	L	219	LYS	5.0
2	L	220	LYS	4.9
2	B	219	LYS	4.9
2	H	220	LYS	4.9
1	I	384	GLY	4.8
1	G	211	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	I	385	VAL	4.7
1	I	383	ARG	4.6
1	G	88	ALA	4.4
1	G	87	THR	4.4
1	I	90	GLY	4.2
1	G	213	LYS	4.2
1	C	210	ASN	4.1
2	J	52	ASN	4.1
2	B	50	GLN	4.0
1	G	154	THR	3.9
1	A	385	VAL	3.9
1	I	390	ILE	3.9
1	G	380	SER	3.8
1	K	117	ASN	3.7
1	I	89	ASN	3.6
1	G	208	PRO	3.6
1	I	386	ALA	3.6
2	F	219	LYS	3.5
2	J	219	LYS	3.4
2	D	220	LYS	3.4
1	K	192	PHE	3.4
1	G	385	VAL	3.4
1	A	382	ASP	3.3
1	E	385	VAL	3.3
1	I	387	SER	3.2
2	J	217	SER	3.2
2	B	49	VAL	3.2
1	A	384	GLY	3.1
1	A	383	ARG	3.1
2	L	216	LEU	3.0
1	G	379	SER	3.0
1	A	386	ALA	3.0
1	C	193	MET	3.0
1	G	206	PHE	2.9
1	I	217	TYR	2.9
1	E	382	ASP	2.9
1	I	394	ILE	2.9
1	C	380	SER	2.8
2	H	50	GLN	2.8
1	K	90	GLY	2.8
1	A	387	SER	2.7
1	C	376	MET	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	217	SER	2.7
1	K	209	LYS	2.6
1	G	381	SER	2.6
1	K	120	LYS	2.6
2	H	49	VAL	2.6
2	F	214	LYS	2.6
1	E	383	ARG	2.6
1	K	217	TYR	2.6
2	D	28	LYS	2.6
1	G	86	PRO	2.6
1	G	386	ALA	2.5
2	D	50	GLN	2.5
1	C	156	GLU	2.5
1	C	209	LYS	2.5
2	J	53	LYS	2.5
1	C	216	LYS	2.5
2	J	213	ALA	2.5
1	C	197	PRO	2.5
2	H	52	ASN	2.4
1	K	91	SER	2.4
1	K	84	LEU	2.4
1	A	217	TYR	2.4
2	J	151	ALA	2.4
1	G	155	ILE	2.4
1	I	397	LEU	2.3
1	G	387	SER	2.3
1	G	116	LEU	2.3
1	G	376	MET	2.3
1	E	390	ILE	2.3
2	H	53	LYS	2.3
1	I	398	ILE	2.3
1	C	374	THR	2.3
1	C	206	PHE	2.3
1	C	187	THR	2.3
1	I	389	MET	2.2
1	G	383	ARG	2.2
1	C	208	PRO	2.2
1	E	386	ALA	2.2
1	C	126	ASN	2.2
1	G	384	GLY	2.2
1	C	207	LEU	2.2
2	B	53	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	153	GLU	2.1
1	G	109	SER	2.1
1	C	186	ALA	2.1
1	E	384	GLY	2.1
1	C	196	LYS	2.1
1	C	184	GLU	2.1
1	C	192	PHE	2.1
1	I	206	PHE	2.0
1	G	126	ASN	2.0
1	A	146	GLY	2.0
1	A	390	ILE	2.0
1	K	127	LEU	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 carbohydrates 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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	EDO	I	501	4/4	0.79	0.25	0.69	31,37,37,40	0

6.5 Other polymers (i)

There are no such residues in this entry.