



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:45 am GMT

PDB ID : 3H8G
Title : Bestatin complex structure of leucine aminopeptidase from *Pseudomonas putida*
Authors : Kale, A.; Dijkstra, B.W.; Sonke, T.; Thunnissen, A.M.W.H.
Deposited on : 2009-04-29
Resolution : 1.50 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

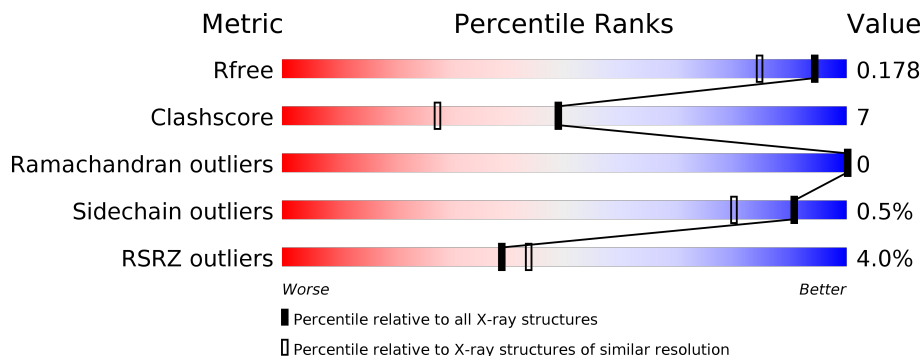
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	100719	2279 (1.50-1.50)
Clashscore	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (1.50-1.50)

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 $\leq 5\%$. 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	497	<div> <div>4%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	B	497	<div> <div>4%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	C	497	<div> <div>4%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	D	497	<div> <div>5%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	E	497	<div> <div>4%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	F	497	<div> <div>3%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25232 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 Cytosol aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	497	Total	C	N	O	S	0	0	0
			3682	2324	644	696	18			
1	A	497	Total	C	N	O	S	0	0	0
			3682	2324	644	696	18			
1	B	497	Total	C	N	O	S	0	0	0
			3678	2322	644	694	18			
1	C	497	Total	C	N	O	S	0	0	0
			3678	2322	644	694	18			
1	D	497	Total	C	N	O	S	0	0	0
			3682	2324	644	696	18			
1	E	497	Total	C	N	O	S	0	0	0
			3682	2324	644	696	18			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

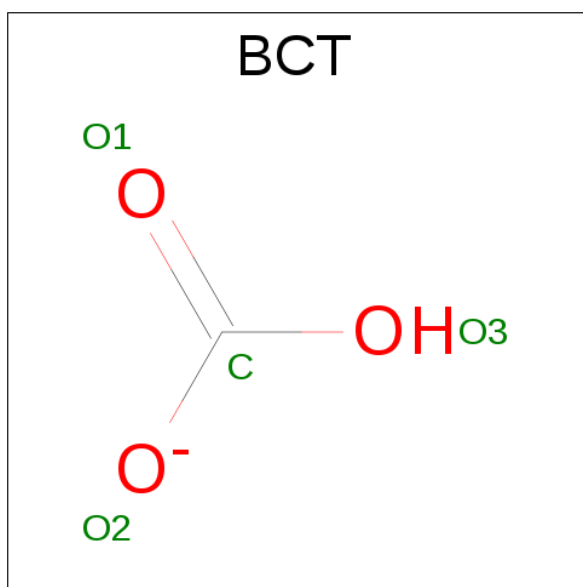
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

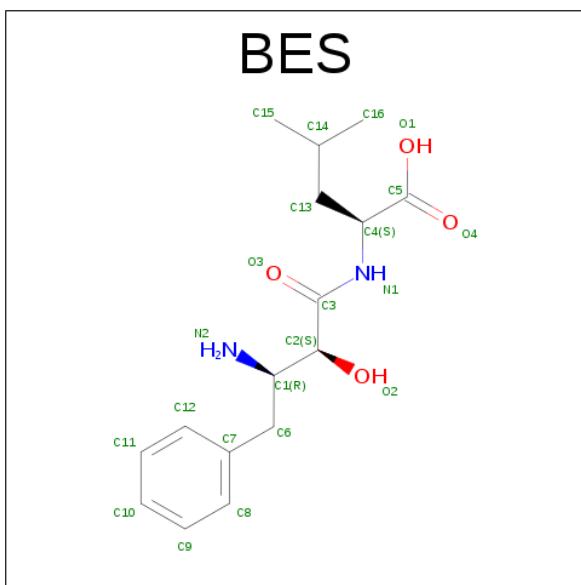
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total K 1 1	0	0
4	E	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	A	1	Total K 1 1	0	0
4	F	1	Total K 1 1	0	0

- Molecule 5 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		
5	B	1	Total	C	O	0	0
			4	1	3		
5	C	1	Total	C	O	0	0
			4	1	3		
5	D	1	Total	C	O	0	0
			4	1	3		
5	E	1	Total	C	O	0	0
			4	1	3		
5	F	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (three-letter code: BES) (formula: C₁₆H₂₄N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			22	16	2	4		
6	B	1	Total	C	N	O	0	0
			22	16	2	4		
6	C	1	Total	C	N	O	0	0
			22	16	2	4		
6	D	1	Total	C	N	O	0	0
			22	16	2	4		
6	E	1	Total	C	N	O	0	0
			22	16	2	4		
6	F	1	Total	C	N	O	0	0
			22	16	2	4		

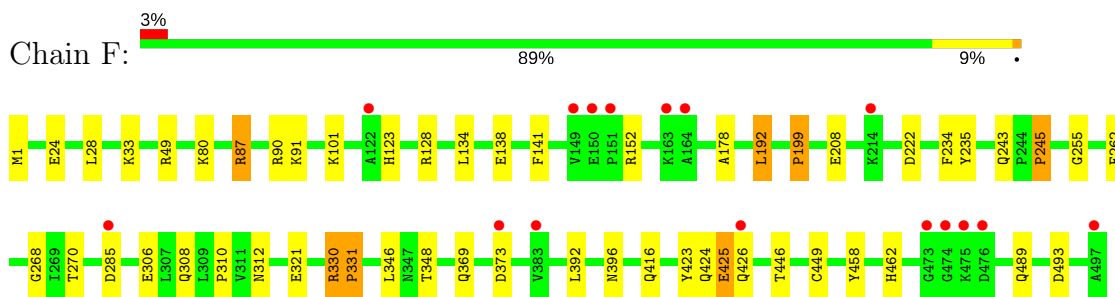
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	480	Total	O	0	0
			480	480		
7	B	511	Total	O	0	0
			511	511		
7	C	488	Total	O	0	0
			488	488		
7	D	481	Total	O	0	0
			481	481		
7	E	491	Total	O	0	0
			491	491		
7	F	523	Total	O	0	0
			523	523		

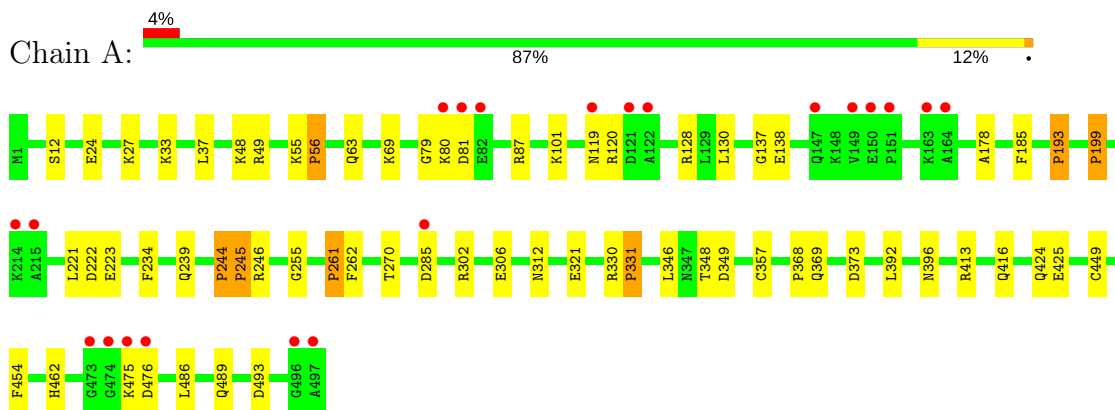
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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.

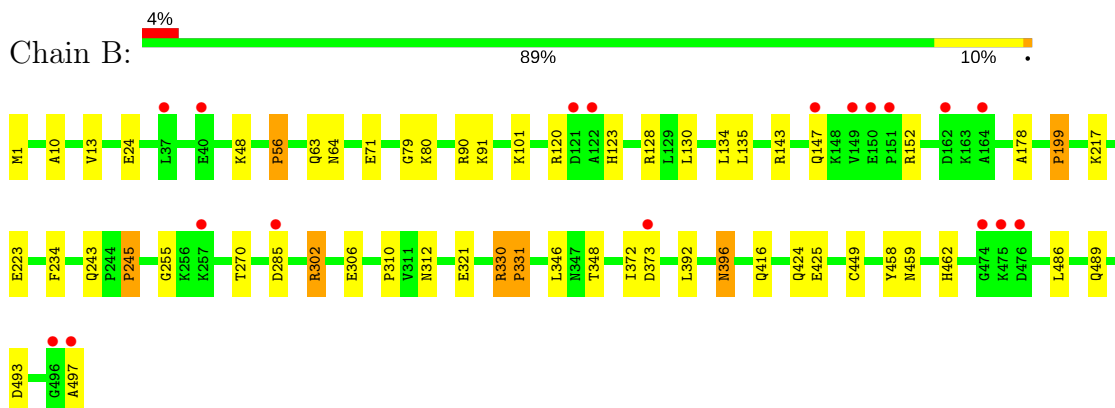
- Molecule 1: Cytosol aminopeptidase



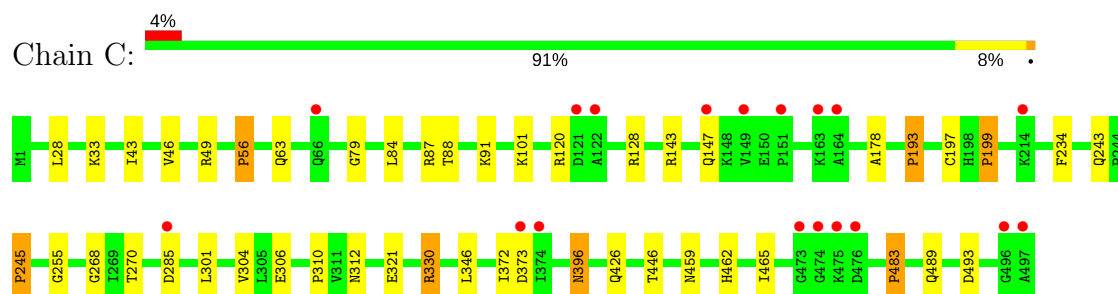
- Molecule 1: Cytosol aminopeptidase



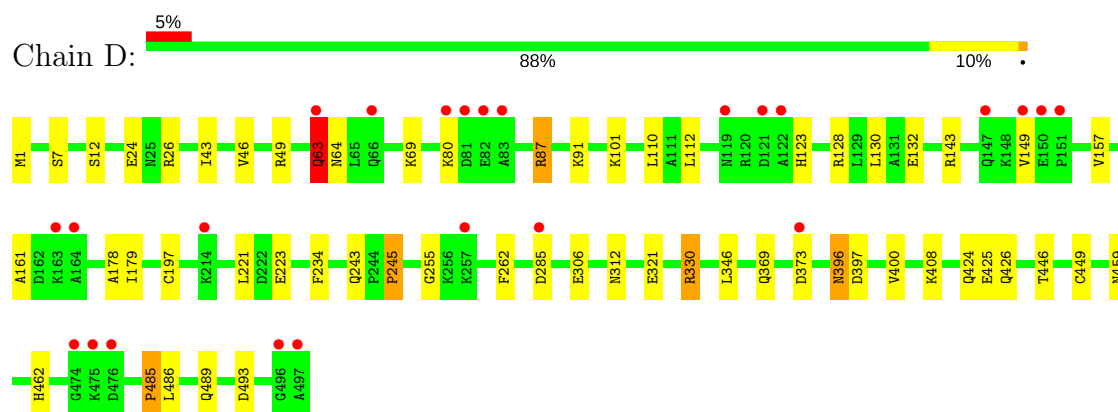
- Molecule 1: Cytosol aminopeptidase



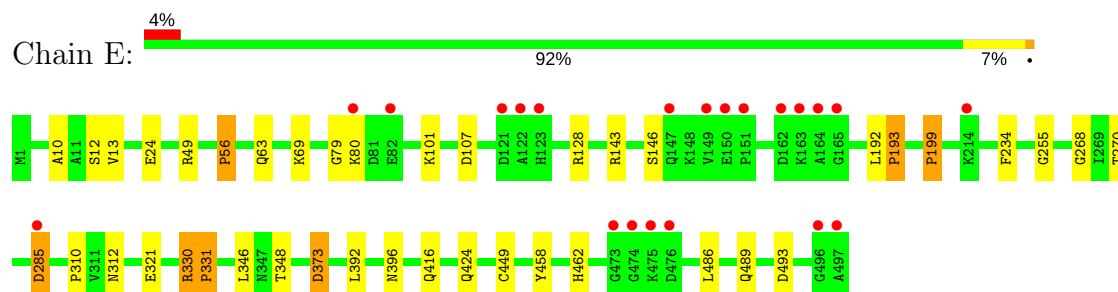
- Molecule 1: Cytosol aminopeptidase



- Molecule 1: Cytosol aminopeptidase



- Molecule 1: Cytosol aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.98Å 95.99Å 96.00Å 100.82° 107.78° 93.23°	Depositor
Resolution (Å)	38.63 – 1.50 38.63 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (38.63-1.50) 88.6 (38.63-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.149 , 0.173 0.160 , 0.178	Depositor DCC
R_{free} test set	24264 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25232	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: BCT, BES, ZN, MN, K

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	0.82	5/3737 (0.1%)	0.90	19/5054 (0.4%)
1	B	0.82	5/3733 (0.1%)	0.86	9/5049 (0.2%)
1	C	0.84	9/3733 (0.2%)	0.88	9/5049 (0.2%)
1	D	0.76	1/3737 (0.0%)	0.83	6/5054 (0.1%)
1	E	0.83	4/3737 (0.1%)	0.87	8/5054 (0.2%)
1	F	0.81	4/3737 (0.1%)	0.88	10/5054 (0.2%)
All	All	0.81	28/22414 (0.1%)	0.87	61/30314 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
All	All	0	5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	245	PRO	N-CD	-9.72	1.34	1.47
1	B	120	ARG	C-N	8.49	1.53	1.34
1	C	483	PRO	N-CD	-7.72	1.37	1.47
1	F	268	GLY	C-O	-7.30	1.11	1.23
1	A	425	GLU	CG-CD	6.72	1.62	1.51
1	C	268	GLY	C-O	-6.67	1.12	1.23
1	C	56	PRO	N-CD	-6.65	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	199	PRO	N-CD	-6.44	1.38	1.47
1	A	245	PRO	N-CD	-6.20	1.39	1.47
1	C	120	ARG	C-N	6.08	1.48	1.34
1	B	245	PRO	N-CD	-5.90	1.39	1.47
1	A	475	LYS	C-N	-5.85	1.20	1.34
1	C	396	ASN	C-N	5.84	1.47	1.34
1	A	476	ASP	C-N	-5.83	1.20	1.34
1	F	235	TYR	CD1-CE1	5.79	1.48	1.39
1	E	146	SER	C-N	-5.78	1.20	1.34
1	B	372	ILE	C-N	-5.73	1.20	1.34
1	A	199	PRO	N-CD	-5.58	1.40	1.47
1	C	372	ILE	C-N	-5.58	1.21	1.34
1	F	425	GLU	CB-CG	-5.54	1.41	1.52
1	F	423	TYR	C-N	5.50	1.46	1.34
1	B	331	PRO	N-CD	-5.47	1.40	1.47
1	E	268	GLY	C-O	-5.38	1.15	1.23
1	E	285	ASP	C-N	-5.37	1.21	1.34
1	B	147	GLN	C-N	-5.35	1.21	1.34
1	E	199	PRO	N-CD	-5.33	1.40	1.47
1	D	197	CYS	C-O	-5.27	1.13	1.23
1	C	197	CYS	C-O	-5.23	1.13	1.23

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	PRO	CA-N-CD	-9.09	98.77	111.50
1	F	310	PRO	CA-N-CD	-8.97	98.94	111.50
1	D	485	PRO	CA-N-CD	-8.89	99.05	111.50
1	A	244	PRO	CA-N-CD	-8.77	99.22	111.50
1	C	56	PRO	CA-N-CD	-8.72	99.28	111.50
1	C	245	PRO	CA-N-CD	-8.72	99.29	111.50
1	E	310	PRO	CA-N-CD	-8.67	99.36	111.50
1	A	261	PRO	CA-N-CD	-8.63	99.42	111.50
1	D	245	PRO	CA-N-CD	-8.43	99.69	111.50
1	B	310	PRO	CA-N-CD	-8.41	99.72	111.50
1	E	56	PRO	CA-N-CD	-8.41	99.73	111.50
1	A	331	PRO	CA-N-CD	-8.38	99.77	111.50
1	A	245	PRO	CA-N-CD	-8.37	99.79	111.50
1	B	56	PRO	CA-N-CD	-8.36	99.80	111.50
1	F	245	PRO	CA-N-CD	-8.35	99.81	111.50
1	B	331	PRO	CA-N-CD	-8.34	99.83	111.50
1	F	199	PRO	CA-N-CD	-8.30	99.89	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	PRO	CA-N-CD	-8.28	99.90	111.50
1	C	199	PRO	CA-N-CD	-8.27	99.92	111.50
1	E	193	PRO	CA-N-CD	-8.24	99.96	111.50
1	A	193	PRO	CA-N-CD	-8.19	100.03	111.50
1	F	331	PRO	CA-N-CD	-8.14	100.11	111.50
1	C	310	PRO	CA-N-CD	-8.12	100.14	111.50
1	A	199	PRO	CA-N-CD	-8.06	100.22	111.50
1	C	396	ASN	O-C-N	7.97	135.45	122.70
1	A	56	PRO	CA-N-CD	-7.96	100.35	111.50
1	E	331	PRO	CA-N-CD	-7.96	100.36	111.50
1	E	199	PRO	CA-N-CD	-7.82	100.55	111.50
1	C	483	PRO	CA-N-CD	-7.80	100.59	111.50
1	B	199	PRO	CA-N-CD	-7.64	100.80	111.50
1	F	192	LEU	O-C-N	7.47	135.29	121.10
1	E	192	LEU	O-C-N	6.51	133.47	121.10
1	D	396	ASN	O-C-N	6.08	132.42	122.70
1	A	120	ARG	O-C-N	-5.96	113.16	122.70
1	A	119	ASN	C-N-CA	5.81	136.23	121.70
1	A	349	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	413	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	396	ASN	CA-C-N	-5.72	104.61	117.20
1	B	396	ASN	O-C-N	5.71	131.83	122.70
1	A	246	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	222	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	425	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	A	185	PHE	CB-CG-CD1	5.38	124.57	120.80
1	F	134	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	A	119	ASN	O-C-N	-5.31	114.20	122.70
1	E	330	ARG	CG-CD-NE	-5.30	100.68	111.80
1	B	302	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	87	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	493	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	493	ASP	CB-CG-OD2	5.21	122.99	118.30
1	F	90	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	493	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	493	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	493	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	87	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	F	493	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	222	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	90	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	F	87	ARG	NE-CZ-NH2	-5.09	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	330	ARG	CG-CD-NE	-5.01	101.28	111.80
1	A	185	PHE	CB-CG-CD2	-5.00	117.30	120.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	GLN	Sidechain
1	B	330	ARG	Sidechain
1	C	330	ARG	Sidechain
1	D	63	GLN	Peptide
1	F	330	ARG	Sidechain

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	3682	0	3776	66	1
1	B	3678	0	3772	64	0
1	C	3678	0	3772	49	0
1	D	3682	0	3777	57	0
1	E	3682	0	3776	49	0
1	F	3682	0	3777	49	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
5	E	4	0	0	0	0
5	F	4	0	0	0	0
6	A	22	0	22	0	0
6	B	22	0	22	0	0
6	C	22	0	22	0	0
6	D	22	0	22	0	0
6	E	22	0	22	0	0
6	F	22	0	22	0	0
7	A	480	0	0	15	0
7	B	511	0	0	14	0
7	C	488	0	0	3	0
7	D	481	0	0	7	0
7	E	491	0	0	9	0
7	F	523	0	0	8	0
All	All	25232	0	22782	306	1

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 7.

All (306) 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:D:101:LYS:HG2	7:D:2782:HOH:O	1.35	1.22
1:E:101:LYS:HG2	7:E:2756:HOH:O	1.36	1.22
1:B:373:ASP:OD1	1:B:462:HIS:HA	1.51	1.09
1:F:373:ASP:OD1	1:F:462:HIS:HA	1.52	1.09
1:D:373:ASP:OD1	1:D:462:HIS:HA	1.54	1.07
1:E:24:GLU:OE1	1:E:80:LYS:HG3	1.54	1.05
1:A:262:PHE:CZ	1:A:369:GLN:NE2	2.24	1.05
1:E:331:PRO:HD3	1:E:348:THR:HG23	1.38	1.04
1:C:373:ASP:OD1	1:C:462:HIS:HA	1.58	1.03
1:D:24:GLU:OE1	1:D:80:LYS:HG3	1.59	1.02
1:B:302:ARG:HD2	7:B:3190:HOH:O	1.58	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:331:PRO:HD3	1:F:348:THR:HG23	1.42	1.02
1:E:101:LYS:HG3	7:E:3011:HOH:O	1.58	1.02
1:A:331:PRO:HD3	1:A:348:THR:HG23	1.38	1.01
1:A:373:ASP:OD1	1:A:462:HIS:HA	1.60	1.01
1:F:262:PHE:CZ	1:F:369:GLN:NE2	2.30	0.99
1:B:331:PRO:HD3	1:B:348:THR:HG23	1.44	0.98
1:B:178:ALA:HA	1:B:306:GLU:OE1	1.64	0.97
1:D:262:PHE:CZ	1:D:369:GLN:NE2	2.31	0.96
1:A:101:LYS:HG2	7:A:2736:HOH:O	1.64	0.95
1:C:178:ALA:HA	1:C:306:GLU:OE1	1.67	0.95
1:D:178:ALA:HA	1:D:306:GLU:OE1	1.72	0.90
1:F:49:ARG:HH21	1:B:63:GLN:HE21	1.18	0.89
1:A:128:ARG:HH12	1:A:489:GLN:HE22	1.19	0.89
1:A:261:PRO:HD2	1:A:368:PRO:HA	1.55	0.89
1:F:128:ARG:HH12	1:F:489:GLN:HE22	1.19	0.88
1:B:199:PRO:HD3	1:B:270:THR:HG21	1.57	0.87
1:E:128:ARG:HH12	1:E:489:GLN:HE22	1.23	0.87
1:C:128:ARG:HH12	1:C:489:GLN:HE22	1.22	0.86
1:B:1:MET:CE	1:B:135:LEU:HD23	2.06	0.86
1:C:199:PRO:HD3	1:C:270:THR:HG21	1.59	0.85
1:C:49:ARG:HH21	1:E:63:GLN:HE21	1.24	0.85
1:A:24:GLU:OE2	7:A:2939:HOH:O	1.97	0.83
1:E:373:ASP:OD1	1:E:462:HIS:HD2	1.61	0.83
1:A:101:LYS:HE2	1:A:138:GLU:OE2	1.79	0.83
1:A:199:PRO:HD3	1:A:270:THR:HG21	1.59	0.83
1:D:128:ARG:HH12	1:D:489:GLN:HE22	1.23	0.82
1:F:199:PRO:HD3	1:F:270:THR:HG21	1.61	0.82
1:F:178:ALA:HA	1:F:306:GLU:OE1	1.79	0.82
1:F:285:ASP:OD2	1:C:346:LEU:HD22	1.79	0.81
1:A:178:ALA:HA	1:A:306:GLU:OE1	1.82	0.80
1:E:24:GLU:OE1	1:E:80:LYS:CG	2.31	0.79
1:B:199:PRO:HD3	1:B:270:THR:CG2	2.12	0.78
1:F:199:PRO:HD3	1:F:270:THR:CG2	2.13	0.78
1:A:101:LYS:HG3	7:A:3082:HOH:O	1.84	0.78
1:E:193:PRO:HD2	1:E:193:PRO:O	1.83	0.78
1:B:48:LYS:HE2	7:B:2904:HOH:O	1.84	0.77
1:E:199:PRO:HD3	1:E:270:THR:HG21	1.65	0.77
1:C:101:LYS:HG3	7:C:2728:HOH:O	1.85	0.77
1:C:193:PRO:HD2	1:C:193:PRO:O	1.85	0.76
1:C:199:PRO:HD3	1:C:270:THR:CG2	2.15	0.76
1:B:128:ARG:HH12	1:B:489:GLN:HE22	1.29	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ASP:OD2	1:E:346:LEU:HD22	1.85	0.76
1:B:346:LEU:HD22	1:E:285:ASP:OD2	1.85	0.75
1:E:107:ASP:CG	7:E:3323:HOH:O	2.23	0.75
1:D:24:GLU:OE1	1:D:80:LYS:CG	2.33	0.75
1:A:193:PRO:O	1:A:193:PRO:HD2	1.86	0.75
1:A:199:PRO:HD3	1:A:270:THR:CG2	2.16	0.75
1:B:1:MET:HE1	1:B:134:LEU:HG	1.67	0.74
1:B:424:GLN:NE2	1:B:449:CYS:SG	2.60	0.74
1:A:346:LEU:HD22	1:C:285:ASP:OD2	1.88	0.74
1:B:24:GLU:OE1	1:B:80:LYS:CG	2.37	0.73
1:B:56:PRO:HD3	1:B:79:GLY:CA	2.19	0.72
1:F:346:LEU:HD22	1:A:285:ASP:OD2	1.89	0.72
1:C:245:PRO:HD2	1:C:245:PRO:O	1.88	0.72
1:E:199:PRO:HD3	1:E:270:THR:CG2	2.20	0.72
1:D:424:GLN:NE2	1:D:449:CYS:SG	2.63	0.72
1:A:331:PRO:HD3	1:A:348:THR:CG2	2.18	0.72
1:C:143:ARG:HD3	7:C:2667:HOH:O	1.89	0.71
1:F:91:LYS:HG3	7:F:3076:HOH:O	1.88	0.71
1:D:426:GLN:OE1	1:D:446:THR:CG2	2.39	0.70
1:B:285:ASP:OD2	1:D:346:LEU:HD22	1.91	0.70
1:E:56:PRO:HD3	1:E:79:GLY:N	2.07	0.70
1:A:244:PRO:HD2	7:A:519:HOH:O	1.92	0.70
1:C:56:PRO:HD3	1:C:79:GLY:CA	2.21	0.69
1:B:24:GLU:OE1	1:B:80:LYS:HG2	1.91	0.69
1:B:424:GLN:HE22	1:B:449:CYS:CB	2.04	0.69
1:B:1:MET:HE3	1:B:135:LEU:HD23	1.73	0.69
1:C:301:LEU:O	1:C:304:VAL:HG12	1.93	0.69
1:A:245:PRO:HD2	1:A:245:PRO:O	1.92	0.69
1:A:244:PRO:HD2	1:A:244:PRO:O	1.91	0.69
1:F:331:PRO:HD3	1:F:348:THR:CG2	2.22	0.69
1:C:49:ARG:HH21	1:E:63:GLN:NE2	1.89	0.69
1:D:245:PRO:O	1:D:245:PRO:HD2	1.93	0.68
1:F:49:ARG:HH21	1:B:63:GLN:NE2	1.88	0.68
1:B:245:PRO:O	1:B:245:PRO:HD2	1.91	0.68
1:B:1:MET:HE3	1:B:135:LEU:CD2	2.23	0.68
1:B:302:ARG:CD	7:B:3190:HOH:O	2.30	0.68
1:C:301:LEU:HA	1:C:304:VAL:HG12	1.74	0.68
1:C:63:GLN:HE21	1:E:49:ARG:HH21	1.39	0.68
1:A:101:LYS:NZ	1:A:137:GLY:O	2.28	0.67
1:E:396:ASN:ND2	7:E:891:HOH:O	2.27	0.67
1:F:426:GLN:OE1	1:F:446:THR:CG2	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:GLU:HG3	7:B:3122:HOH:O	1.95	0.67
1:C:33:LYS:HE3	7:C:3312:HOH:O	1.93	0.67
1:D:462:HIS:HE1	7:D:509:HOH:O	1.78	0.67
1:F:1:MET:CE	1:F:138:GLU:OE2	2.43	0.66
1:A:24:GLU:OE1	1:A:80:LYS:HG3	1.96	0.66
1:A:56:PRO:HD3	1:A:79:GLY:N	2.10	0.66
1:C:56:PRO:HD3	1:C:79:GLY:N	2.11	0.66
1:C:373:ASP:OD1	1:C:462:HIS:CA	2.42	0.66
1:D:397:ASP:HA	1:D:400:VAL:HG22	1.76	0.66
1:A:49:ARG:CZ	7:A:3199:HOH:O	2.44	0.65
1:B:331:PRO:HD3	1:B:348:THR:CG2	2.22	0.65
1:B:462:HIS:HE1	7:B:514:HOH:O	1.80	0.65
1:F:396:ASN:ND2	7:F:780:HOH:O	2.27	0.65
1:B:424:GLN:NE2	1:B:449:CYS:HB3	2.12	0.65
1:F:285:ASP:OD2	1:C:346:LEU:CD2	2.45	0.64
1:B:424:GLN:NE2	1:B:449:CYS:CB	2.60	0.64
1:A:462:HIS:HE1	7:A:528:HOH:O	1.81	0.64
1:E:462:HIS:HE1	7:E:537:HOH:O	1.81	0.64
1:A:396:ASN:ND2	7:A:1195:HOH:O	2.30	0.63
1:B:373:ASP:OD1	1:B:462:HIS:CA	2.39	0.63
7:A:976:HOH:O	1:C:147:GLN:HG2	1.99	0.62
1:E:56:PRO:HD3	1:E:79:GLY:CA	2.30	0.62
1:A:261:PRO:O	1:A:261:PRO:HD2	1.98	0.62
1:B:91:LYS:HG3	7:B:3363:HOH:O	1.98	0.62
1:A:49:ARG:HH21	1:D:63:GLN:HE21	1.47	0.62
1:D:179:ILE:HG23	1:D:485:PRO:HD3	1.82	0.62
1:F:245:PRO:HD2	1:F:245:PRO:O	1.98	0.62
1:A:424:GLN:NE2	1:A:449:CYS:SG	2.72	0.61
1:F:24:GLU:OE1	1:F:80:LYS:HG3	2.00	0.61
1:E:331:PRO:HD3	1:E:348:THR:CG2	2.21	0.60
1:D:132:GLU:OE2	1:D:485:PRO:HG3	2.00	0.60
1:E:24:GLU:OE1	1:E:80:LYS:HE3	2.02	0.60
1:B:1:MET:HE2	1:B:135:LEU:HD23	1.84	0.60
1:D:426:GLN:OE1	1:D:446:THR:HG21	2.01	0.60
1:D:373:ASP:OD1	1:D:462:HIS:CA	2.42	0.60
1:D:424:GLN:HE22	1:D:449:CYS:CB	2.15	0.59
1:A:56:PRO:HD3	1:A:79:GLY:CA	2.32	0.59
1:A:424:GLN:NE2	1:A:449:CYS:HB3	2.16	0.59
1:B:424:GLN:HE22	1:B:449:CYS:HB3	1.66	0.59
1:B:321:GLU:OE2	1:D:330:ARG:HD3	2.01	0.59
1:C:49:ARG:NH2	1:E:63:GLN:HE21	1.96	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:LEU:O	1:C:304:VAL:CG1	2.50	0.59
1:D:285:ASP:OD2	1:E:346:LEU:CD2	2.50	0.59
1:F:346:LEU:CD2	1:A:285:ASP:OD2	2.51	0.58
1:D:424:GLN:NE2	1:D:449:CYS:CB	2.67	0.58
1:D:424:GLN:NE2	1:D:449:CYS:HB3	2.18	0.58
1:B:101:LYS:HG3	1:B:152:ARG:HD3	1.86	0.58
1:D:425:GLU:HG3	7:D:2857:HOH:O	2.04	0.58
1:F:255:GLY:H	1:F:312:ASN:ND2	2.02	0.58
1:B:56:PRO:HD3	1:B:79:GLY:N	2.19	0.58
1:C:465:ILE:HG21	1:C:483:PRO:HG3	1.86	0.58
1:E:255:GLY:H	1:E:312:ASN:ND2	2.01	0.58
1:B:1:MET:CE	1:B:135:LEU:CD2	2.80	0.58
1:F:24:GLU:OE1	1:F:80:LYS:CG	2.52	0.58
1:F:87:ARG:HG3	1:F:91:LYS:HE2	1.86	0.58
1:B:24:GLU:OE1	1:B:80:LYS:HG3	2.02	0.57
1:B:396:ASN:HD22	1:B:459:ASN:ND2	2.02	0.57
1:C:301:LEU:HA	1:C:304:VAL:CG1	2.34	0.57
1:D:87:ARG:HG3	1:D:91:LYS:HE2	1.86	0.57
1:F:123:HIS:HE1	7:F:2725:HOH:O	1.87	0.57
1:F:101:LYS:HG3	1:F:152:ARG:CD	2.35	0.57
1:F:373:ASP:OD1	1:F:462:HIS:CA	2.39	0.57
1:A:261:PRO:CD	1:A:368:PRO:HA	2.32	0.57
1:C:199:PRO:CD	1:C:270:THR:HG21	2.34	0.57
1:F:425:GLU:HG3	7:F:3119:HOH:O	2.04	0.57
1:C:28:LEU:O	1:C:33:LYS:HE2	2.05	0.57
1:E:424:GLN:NE2	1:E:449:CYS:SG	2.78	0.57
1:F:128:ARG:HH12	1:F:489:GLN:NE2	1.98	0.57
1:D:123:HIS:HE1	7:D:2762:HOH:O	1.87	0.57
1:A:424:GLN:HE22	1:A:449:CYS:CB	2.18	0.56
1:A:346:LEU:CD2	1:C:285:ASP:OD2	2.53	0.56
1:A:424:GLN:NE2	1:A:449:CYS:CB	2.69	0.56
1:F:308:GLN:HG2	7:F:2739:HOH:O	2.06	0.56
1:F:426:GLN:OE1	1:F:446:THR:HG21	2.06	0.56
1:E:373:ASP:OD1	1:E:462:HIS:CD2	2.51	0.56
1:A:255:GLY:H	1:A:312:ASN:ND2	2.04	0.55
1:A:24:GLU:OE1	1:A:80:LYS:CG	2.55	0.55
1:A:373:ASP:OD1	1:A:462:HIS:CA	2.47	0.55
1:B:1:MET:CE	1:B:134:LEU:HG	2.36	0.55
1:E:24:GLU:CD	1:E:80:LYS:HG3	2.24	0.55
1:C:301:LEU:CA	1:C:304:VAL:HG12	2.37	0.55
1:C:396:ASN:HD22	1:C:459:ASN:ND2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:GLN:NE2	1:E:49:ARG:HH21	2.05	0.54
1:F:33:LYS:HE3	7:F:3133:HOH:O	2.07	0.54
1:D:24:GLU:CD	1:D:80:LYS:HG3	2.28	0.54
1:F:1:MET:HE3	1:F:138:GLU:OE2	2.08	0.54
1:C:63:GLN:HE21	1:E:49:ARG:NH2	2.06	0.54
1:E:424:GLN:NE2	1:E:449:CYS:HB3	2.23	0.54
1:D:321:GLU:OE2	1:E:330:ARG:HD3	2.08	0.53
1:B:285:ASP:OD2	1:D:346:LEU:CD2	2.56	0.53
1:D:397:ASP:HA	1:D:400:VAL:CG2	2.38	0.53
1:C:426:GLN:OE1	1:C:446:THR:HG21	2.09	0.53
1:B:255:GLY:H	1:B:312:ASN:ND2	2.07	0.53
1:B:48:LYS:CE	7:B:2904:HOH:O	2.50	0.52
1:A:424:GLN:HE22	1:A:449:CYS:HB3	1.75	0.52
1:D:43:ILE:O	1:D:46:VAL:HG22	2.10	0.52
1:E:424:GLN:NE2	1:E:449:CYS:CB	2.73	0.52
1:F:199:PRO:CD	1:F:270:THR:HG21	2.36	0.52
1:A:27:LYS:NZ	1:A:81:ASP:OD2	2.43	0.52
1:B:396:ASN:HD22	1:B:459:ASN:CG	2.13	0.52
1:D:110:LEU:HB3	1:D:112:LEU:HD13	1.91	0.52
1:B:346:LEU:CD2	1:E:285:ASP:OD2	2.56	0.52
1:C:193:PRO:CD	1:C:193:PRO:O	2.57	0.52
1:D:396:ASN:HD22	1:D:459:ASN:ND2	2.08	0.52
1:F:101:LYS:HG3	1:F:152:ARG:HD3	1.92	0.52
1:C:56:PRO:CD	1:C:79:GLY:CA	2.87	0.51
1:E:193:PRO:CD	1:E:193:PRO:O	2.55	0.51
1:F:330:ARG:HD3	1:A:321:GLU:OE2	2.10	0.51
1:F:424:GLN:NE2	1:F:449:CYS:SG	2.83	0.51
1:A:331:PRO:CD	1:A:348:THR:HG23	2.26	0.51
1:A:199:PRO:CD	1:A:270:THR:HG21	2.37	0.51
1:F:128:ARG:NH1	1:F:489:GLN:HE22	2.00	0.51
1:A:49:ARG:NE	7:A:3199:HOH:O	2.43	0.51
1:E:331:PRO:CD	1:E:348:THR:HG23	2.25	0.50
1:F:152:ARG:CZ	7:F:2813:HOH:O	2.59	0.50
1:B:101:LYS:HG3	1:B:152:ARG:CD	2.42	0.50
1:D:255:GLY:H	1:D:312:ASN:ND2	2.09	0.50
1:F:28:LEU:O	1:F:33:LYS:HE2	2.12	0.50
1:A:55:LYS:HE2	7:A:575:HOH:O	2.10	0.49
1:D:64:ASN:N	1:D:64:ASN:OD1	2.44	0.49
1:B:143:ARG:HD3	7:B:2662:HOH:O	2.12	0.49
1:B:71:GLU:OE1	7:B:607:HOH:O	2.20	0.49
1:C:255:GLY:H	1:C:312:ASN:ND2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:LEU:N	1:D:221:LEU:HD12	2.28	0.49
1:C:396:ASN:HD22	1:C:459:ASN:CG	2.16	0.48
1:D:149:VAL:O	1:D:149:VAL:HG23	2.12	0.48
1:B:64:ASN:OD1	7:B:1278:HOH:O	2.20	0.48
1:D:143:ARG:HD3	7:D:2695:HOH:O	2.12	0.48
1:D:408:LYS:NZ	7:D:2542:HOH:O	2.44	0.48
1:C:301:LEU:C	1:C:304:VAL:HG12	2.33	0.48
1:A:330:ARG:HD3	1:C:321:GLU:OE2	2.12	0.48
1:E:10:ALA:O	1:E:13:VAL:HG22	2.12	0.48
1:F:101:LYS:HG3	1:F:152:ARG:HD2	1.95	0.48
1:D:128:ARG:HH12	1:D:489:GLN:NE2	2.02	0.48
1:F:424:GLN:NE2	1:F:449:CYS:HB3	2.29	0.48
1:B:199:PRO:CD	1:B:270:THR:HG21	2.37	0.48
1:E:128:ARG:HH12	1:E:489:GLN:NE2	2.03	0.48
1:D:396:ASN:HD22	1:D:459:ASN:CG	2.16	0.47
1:A:128:ARG:HH12	1:A:489:GLN:NE2	2.01	0.47
1:B:392:LEU:O	1:B:416:GLN:HA	2.15	0.47
1:E:424:GLN:HE22	1:E:449:CYS:CB	2.27	0.47
1:F:308:GLN:HG2	7:F:2901:HOH:O	2.13	0.47
1:D:223:GLU:HB2	1:D:245:PRO:CD	2.45	0.47
1:F:24:GLU:CD	1:F:80:LYS:HG3	2.34	0.47
1:B:223:GLU:HB2	1:B:245:PRO:CD	2.44	0.46
1:E:101:LYS:CG	7:E:2756:HOH:O	2.19	0.46
1:B:10:ALA:O	1:B:13:VAL:HG12	2.15	0.46
1:D:424:GLN:HE22	1:D:449:CYS:HB3	1.76	0.46
1:C:63:GLN:HG2	7:E:1354:HOH:O	2.14	0.46
1:D:397:ASP:CA	1:D:400:VAL:HG22	2.45	0.46
1:B:123:HIS:HE1	7:B:2817:HOH:O	1.99	0.46
1:B:48:LYS:HE3	7:B:3233:HOH:O	2.16	0.46
1:B:128:ARG:HH12	1:B:489:GLN:NE2	2.06	0.46
1:E:101:LYS:HE2	7:E:3011:HOH:O	2.16	0.45
1:A:12:SER:O	1:A:69:LYS:HD3	2.17	0.45
1:A:101:LYS:CG	7:A:3082:HOH:O	2.55	0.45
1:A:193:PRO:O	1:A:193:PRO:CD	2.60	0.45
1:D:486:LEU:C	1:D:486:LEU:HD23	2.37	0.45
1:B:56:PRO:CD	1:B:79:GLY:CA	2.93	0.45
1:E:56:PRO:CD	1:E:79:GLY:CA	2.94	0.45
1:A:244:PRO:O	1:A:244:PRO:CD	2.63	0.45
1:A:37:LEU:HD23	7:A:2835:HOH:O	2.18	0.44
1:A:101:LYS:NZ	1:A:137:GLY:C	2.71	0.44
1:D:149:VAL:O	1:D:149:VAL:CG2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:424:GLN:NE2	1:F:449:CYS:CB	2.80	0.44
1:C:128:ARG:HH12	1:C:489:GLN:NE2	2.02	0.44
1:C:245:PRO:CD	1:C:245:PRO:O	2.64	0.44
1:D:12:SER:O	1:D:69:LYS:HD3	2.18	0.44
1:C:426:GLN:OE1	1:C:446:THR:CG2	2.65	0.44
1:A:302:ARG:HG3	7:A:2987:HOH:O	2.18	0.44
1:B:1:MET:HE3	1:B:135:LEU:HD21	1.98	0.44
1:F:243:GLN:HB2	1:F:321:GLU:OE1	2.17	0.43
1:A:48:LYS:HE2	7:A:3158:HOH:O	2.18	0.43
1:C:43:ILE:O	1:C:46:VAL:HG22	2.18	0.43
1:F:141:PHE:HZ	1:F:192:LEU:HD23	1.83	0.43
1:C:87:ARG:HG3	1:C:91:LYS:HE3	2.00	0.43
1:C:84:LEU:HD22	1:C:88:THR:HG21	2.00	0.43
1:C:243:GLN:HB2	1:C:321:GLU:OE1	2.18	0.43
1:D:243:GLN:HB2	1:D:321:GLU:OE1	2.19	0.43
1:E:143:ARG:HB2	1:E:143:ARG:HE	1.43	0.43
1:D:245:PRO:O	1:D:245:PRO:CD	2.65	0.43
1:B:330:ARG:HD3	1:E:321:GLU:OE2	2.19	0.43
1:A:101:LYS:HE3	7:A:3082:HOH:O	2.19	0.43
1:A:128:ARG:NH1	1:A:489:GLN:HE22	2.01	0.43
1:A:486:LEU:HD23	1:A:486:LEU:C	2.40	0.42
1:B:497:ALA:HB2	7:B:3407:HOH:O	2.19	0.42
1:A:223:GLU:HB2	1:A:245:PRO:CD	2.49	0.42
1:E:486:LEU:C	1:E:486:LEU:HD23	2.40	0.42
1:E:107:ASP:CB	7:E:3323:HOH:O	2.68	0.42
1:B:24:GLU:CD	1:B:80:LYS:HG3	2.40	0.42
1:D:130:LEU:C	1:D:130:LEU:HD23	2.40	0.42
1:E:12:SER:O	1:E:69:LYS:HD3	2.19	0.42
1:A:130:LEU:HD23	1:A:130:LEU:C	2.40	0.42
1:A:392:LEU:O	1:A:416:GLN:HA	2.20	0.42
1:B:486:LEU:HD23	1:B:486:LEU:C	2.40	0.41
1:A:221:LEU:N	1:A:221:LEU:HD12	2.35	0.41
1:B:217:LYS:HD3	7:B:671:HOH:O	2.19	0.41
1:B:243:GLN:HB2	1:B:321:GLU:OE1	2.20	0.41
1:D:1:MET:HE3	1:D:157:VAL:HB	2.02	0.41
1:B:130:LEU:C	1:B:130:LEU:HD23	2.40	0.41
1:A:63:GLN:NE2	1:D:49:ARG:NH2	2.69	0.41
1:D:7:SER:HA	1:D:161:ALA:O	2.21	0.41
1:F:321:GLU:OE2	1:C:330:ARG:HD3	2.20	0.41
1:D:223:GLU:HB2	1:D:245:PRO:HD2	2.03	0.41
1:F:392:LEU:O	1:F:416:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LEU:N	1:D:112:LEU:HD12	2.35	0.41
1:D:26:ARG:HD3	7:D:2720:HOH:O	2.20	0.41
1:A:331:PRO:CD	1:A:348:THR:CG2	2.95	0.40
1:A:262:PHE:HZ	1:A:369:GLN:NE2	2.06	0.40
1:E:392:LEU:O	1:E:416:GLN:HA	2.20	0.40
1:E:199:PRO:CD	1:E:270:THR:HG21	2.44	0.40
1:A:357:CYS:HB2	1:A:454:PHE:CG	2.56	0.40
1:F:24:GLU:OE1	1:F:80:LYS:HG2	2.21	0.40

All (1) 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)
1:F:208:GLU:OE2	1:A:33:LYS:NZ[1_655]	1.81	0.39

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	495/497 (100%)	485 (98%)	10 (2%)	0	100	100
1	B	495/497 (100%)	485 (98%)	10 (2%)	0	100	100
1	C	495/497 (100%)	485 (98%)	10 (2%)	0	100	100
1	D	495/497 (100%)	485 (98%)	10 (2%)	0	100	100
1	E	495/497 (100%)	485 (98%)	10 (2%)	0	100	100
1	F	495/497 (100%)	482 (97%)	13 (3%)	0	100	100
All	All	2970/2982 (100%)	2907 (98%)	63 (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	378/378 (100%)	377 (100%)	1 (0%)	94	86
1	B	377/378 (100%)	375 (100%)	2 (0%)	91	80
1	C	377/378 (100%)	376 (100%)	1 (0%)	94	86
1	D	378/378 (100%)	376 (100%)	2 (0%)	91	80
1	E	378/378 (100%)	375 (99%)	3 (1%)	85	68
1	F	378/378 (100%)	376 (100%)	2 (0%)	91	80
All	All	2266/2268 (100%)	2255 (100%)	11 (0%)	91	80

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	234	PHE
1	F	458	TYR
1	A	234	PHE
1	B	234	PHE
1	B	458	TYR
1	C	234	PHE
1	D	63	GLN
1	D	234	PHE
1	E	234	PHE
1	E	373	ASP
1	E	458	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	63	GLN
1	F	123	HIS
1	F	312	ASN
1	F	424	GLN
1	F	489	GLN
1	A	63	GLN

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Mol	Chain	Res	Type
1	A	123	HIS
1	A	312	ASN
1	A	424	GLN
1	A	426	GLN
1	A	462	HIS
1	A	489	GLN
1	B	63	GLN
1	B	123	HIS
1	B	312	ASN
1	B	424	GLN
1	B	426	GLN
1	B	459	ASN
1	B	462	HIS
1	B	489	GLN
1	C	63	GLN
1	C	312	ASN
1	C	459	ASN
1	C	489	GLN
1	D	63	GLN
1	D	123	HIS
1	D	312	ASN
1	D	424	GLN
1	D	459	ASN
1	D	462	HIS
1	D	489	GLN
1	E	63	GLN
1	E	308	GLN
1	E	312	ASN
1	E	369	GLN
1	E	424	GLN
1	E	426	GLN
1	E	462	HIS
1	E	489	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 18 are monoatomic - leaving 12 for Mogul analysis.

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	$\# Z > 2$
5	BCT	A	504	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BES	A	505	3,2	19,22,22	0.74	0	19,29,29	1.53	5 (26%)
5	BCT	B	504	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BES	B	505	3,2	19,22,22	0.87	1 (5%)	19,29,29	1.25	2 (10%)
5	BCT	C	504	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BES	C	505	3,2	19,22,22	1.08	2 (10%)	19,29,29	1.27	2 (10%)
5	BCT	D	504	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BES	D	505	3,2	19,22,22	0.92	0	19,29,29	1.24	2 (10%)
5	BCT	E	504	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BES	E	505	3,2	19,22,22	0.99	2 (10%)	19,29,29	1.35	3 (15%)
5	BCT	F	504	-	0,3,3	0.00	-	0,3,3	0.00	-
6	BES	F	505	3,2	19,22,22	0.88	0	19,29,29	1.55	4 (21%)

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
5	BCT	A	504	-	-	0/0/0/0	0/0/0/0
6	BES	A	505	3,2	-	0/20/24/24	0/1/1/1
5	BCT	B	504	-	-	0/0/0/0	0/0/0/0
6	BES	B	505	3,2	-	0/20/24/24	0/1/1/1
5	BCT	C	504	-	-	0/0/0/0	0/0/0/0
6	BES	C	505	3,2	-	0/20/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCT	D	504	-	-	0/0/0/0	0/0/0/0
6	BES	D	505	3,2	-	0/20/24/24	0/1/1/1
5	BCT	E	504	-	-	0/0/0/0	0/0/0/0
6	BES	E	505	3,2	-	0/20/24/24	0/1/1/1
5	BCT	F	504	-	-	0/0/0/0	0/0/0/0
6	BES	F	505	3,2	-	0/20/24/24	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	505	BES	C2-C3	-2.54	1.47	1.52
6	E	505	BES	C2-C3	-2.35	1.47	1.52
6	B	505	BES	O2-C2	2.06	1.46	1.42
6	E	505	BES	O2-C2	2.42	1.47	1.42
6	C	505	BES	O2-C2	2.45	1.47	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	505	BES	C4-N1-C3	-2.92	118.70	123.16
6	F	505	BES	C4-N1-C3	-2.82	118.85	123.16
6	A	505	BES	C4-N1-C3	-2.81	118.87	123.16
6	A	505	BES	C6-C7-C12	-2.67	115.51	120.91
6	F	505	BES	C6-C7-C12	-2.67	115.51	120.91
6	B	505	BES	O2-C2-C3	-2.43	105.22	110.59
6	D	505	BES	C4-N1-C3	-2.38	119.53	123.16
6	F	505	BES	C11-C12-C7	-2.28	117.17	120.64
6	C	505	BES	C6-C7-C12	-2.27	116.33	120.91
6	E	505	BES	C6-C7-C12	-2.10	116.67	120.91
6	C	505	BES	O2-C2-C3	-2.03	106.11	110.59
6	A	505	BES	C9-C8-C7	-2.01	117.57	120.64
6	A	505	BES	C11-C10-C9	2.07	123.34	119.89
6	E	505	BES	C12-C7-C8	2.11	121.51	118.16
6	B	505	BES	C12-C7-C8	2.25	121.73	118.16
6	D	505	BES	C11-C10-C9	2.39	123.86	119.89
6	A	505	BES	C12-C7-C8	2.47	122.08	118.16
6	F	505	BES	C12-C7-C8	3.37	123.51	118.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	497/497 (100%)	0.06	21 (4%)	37 41	4, 10, 25, 43	0
1	B	497/497 (100%)	0.05	18 (3%)	43 49	5, 9, 23, 35	0
1	C	497/497 (100%)	0.06	18 (3%)	43 49	5, 10, 23, 37	0
1	D	497/497 (100%)	0.07	24 (4%)	31 35	5, 10, 25, 42	0
1	E	497/497 (100%)	-0.01	21 (4%)	37 41	5, 9, 23, 39	0
1	F	497/497 (100%)	-0.04	16 (3%)	48 54	4, 9, 22, 38	0
All	All	2982/2982 (100%)	0.03	118 (3%)	39 44	4, 10, 24, 43	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	475	LYS	6.4
1	A	149	VAL	6.4
1	C	149	VAL	6.0
1	B	475	LYS	5.8
1	D	149	VAL	5.7
1	C	497	ALA	5.5
1	B	149	VAL	5.3
1	A	147	GLN	4.9
1	A	81	ASP	4.8
1	F	475	LYS	4.8
1	E	497	ALA	4.7
1	B	497	ALA	4.5
1	A	214	LYS	4.4
1	D	150	GLU	4.4
1	B	150	GLU	4.3
1	E	163	LYS	4.2
1	D	81	ASP	4.2
1	E	149	VAL	4.2
1	E	151	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	150	GLU	4.2
1	A	475	LYS	4.1
1	D	497	ALA	4.1
1	B	496	GLY	4.0
1	D	475	LYS	4.0
1	F	122	ALA	3.9
1	A	122	ALA	3.9
1	E	475	LYS	3.9
1	C	147	GLN	3.8
1	A	119	ASN	3.7
1	C	121	ASP	3.7
1	B	474	GLY	3.6
1	E	164	ALA	3.6
1	B	151	PRO	3.5
1	E	150	GLU	3.5
1	F	149	VAL	3.5
1	E	122	ALA	3.4
1	F	497	ALA	3.4
1	A	150	GLU	3.4
1	B	147	GLN	3.4
1	D	147	GLN	3.3
1	B	121	ASP	3.3
1	D	82	GLU	3.3
1	D	214	LYS	3.3
1	E	162	ASP	3.2
1	C	476	ASP	3.2
1	C	496	GLY	3.2
1	A	163	LYS	3.2
1	C	122	ALA	3.2
1	D	80	LYS	3.2
1	D	63	GLN	3.1
1	A	497	ALA	3.1
1	F	151	PRO	3.0
1	A	80	LYS	3.0
1	E	147	GLN	3.0
1	B	476	ASP	3.0
1	C	151	PRO	3.0
1	A	474	GLY	2.9
1	E	476	ASP	2.9
1	C	373	ASP	2.9
1	E	496	GLY	2.9
1	B	122	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	83	ALA	2.8
1	D	122	ALA	2.8
1	E	121	ASP	2.8
1	A	164	ALA	2.7
1	C	474	GLY	2.7
1	C	214	LYS	2.7
1	D	476	ASP	2.7
1	C	473	GLY	2.7
1	E	474	GLY	2.7
1	A	82	GLU	2.7
1	A	215	ALA	2.7
1	D	164	ALA	2.7
1	A	121	ASP	2.6
1	A	473	GLY	2.6
1	E	214	LYS	2.6
1	B	285	ASP	2.5
1	D	257	LYS	2.5
1	D	496	GLY	2.5
1	D	119	ASN	2.5
1	B	162	ASP	2.5
1	F	214	LYS	2.5
1	D	163	LYS	2.5
1	E	80	LYS	2.5
1	F	476	ASP	2.4
1	A	151	PRO	2.4
1	B	164	ALA	2.4
1	D	285	ASP	2.4
1	A	496	GLY	2.4
1	C	66	GLN	2.4
1	C	164	ALA	2.4
1	B	373	ASP	2.3
1	A	285	ASP	2.3
1	E	473	GLY	2.3
1	D	373	ASP	2.3
1	D	121	ASP	2.3
1	B	37	LEU	2.2
1	B	40	GLU	2.2
1	F	163	LYS	2.2
1	C	163	LYS	2.2
1	A	476	ASP	2.2
1	C	285	ASP	2.2
1	D	66	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	164	ALA	2.1
1	B	257	LYS	2.1
1	E	165	GLY	2.1
1	F	473	GLY	2.1
1	C	374	ILE	2.1
1	F	373	ASP	2.1
1	F	285	ASP	2.1
1	E	285	ASP	2.1
1	D	151	PRO	2.0
1	E	82	GLU	2.0
1	F	383	VAL	2.0
1	D	474	GLY	2.0
1	F	426	GLN	2.0
1	F	474	GLY	2.0
1	E	123	HIS	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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	BES	F	505	22/22	0.97	0.08	0.26	4,12,17,19	0
2	ZN	C	501	1/1	1.00	0.09	-0.04	6,6,6,6	1
6	BES	B	505	22/22	0.96	0.08	-0.05	5,11,17,19	0
6	BES	A	505	22/22	0.97	0.07	-0.19	4,11,18,22	0
6	BES	D	505	22/22	0.96	0.08	-0.22	6,12,17,20	0
2	ZN	D	501	1/1	1.00	0.07	-0.41	6,6,6,6	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	BES	C	505	22/22	0.97	0.07	-0.53	5,12,17,19	0
2	ZN	A	501	1/1	1.00	0.06	-0.61	5,5,5,5	1
2	ZN	F	501	1/1	1.00	0.07	-0.61	6,6,6,6	1
2	ZN	B	501	1/1	1.00	0.07	-0.65	6,6,6,6	1
6	BES	E	505	22/22	0.98	0.06	-0.89	5,13,17,20	0
2	ZN	E	501	1/1	1.00	0.07	-0.97	6,6,6,6	1
5	BCT	A	504	4/4	0.99	0.05	-1.29	6,6,7,8	0
5	BCT	D	504	4/4	0.99	0.06	-1.56	6,6,7,8	0
5	BCT	B	504	4/4	0.99	0.06	-1.57	7,7,7,8	0
3	MN	C	502	1/1	1.00	0.05	-1.81	5,5,5,5	0
3	MN	B	502	1/1	1.00	0.05	-1.85	6,6,6,6	0
5	BCT	C	504	4/4	0.99	0.05	-1.96	6,7,7,7	0
4	K	C	503	1/1	1.00	0.05	-2.33	6,6,6,6	0
4	K	A	503	1/1	1.00	0.05	-2.39	6,6,6,6	0
5	BCT	F	504	4/4	0.99	0.04	-2.45	6,7,7,8	0
5	BCT	E	504	4/4	0.99	0.04	-2.61	5,6,7,7	0
4	K	D	503	1/1	1.00	0.05	-2.70	6,6,6,6	0
4	K	B	503	1/1	1.00	0.04	-2.76	6,6,6,6	0
3	MN	A	502	1/1	1.00	0.05	-2.77	5,5,5,5	0
4	K	E	503	1/1	1.00	0.03	-2.86	6,6,6,6	0
3	MN	D	502	1/1	1.00	0.04	-3.26	5,5,5,5	0
3	MN	E	502	1/1	1.00	0.04	-3.27	5,5,5,5	0
4	K	F	503	1/1	1.00	0.03	-3.91	6,6,6,6	0
3	MN	F	502	1/1	1.00	0.04	-4.20	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.