Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:07 AM GMT

PDB ID	:	3H8F
Title	:	High pH native 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	:	2.20 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:

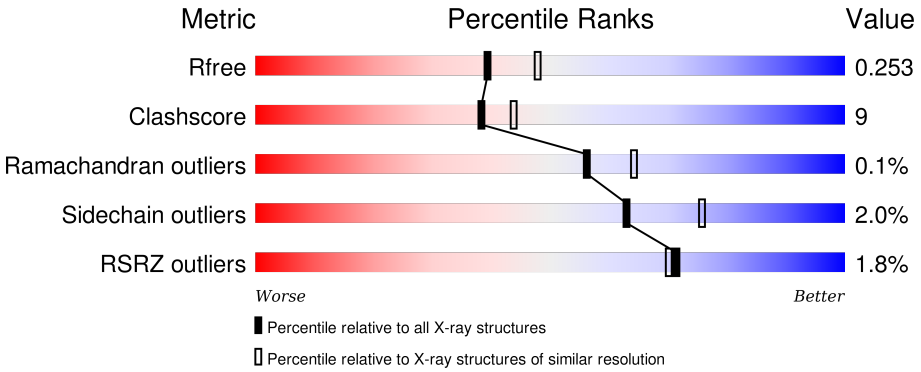
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	497	3% 84% 15%
1	B	497	% 84% 14%
1	C	497	84% 15%
1	D	497	2% 84% 14%
1	E	497	3% 85% 13%

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Mol	Chain	Length	Quality of chain
1	F	497	2% 82% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCT	E	504	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22836 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	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
			3682	2324	644	696	18			
1	C	497	Total	C	N	O	S	0	0	0
			3682	2324	644	696	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			
1	F	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		

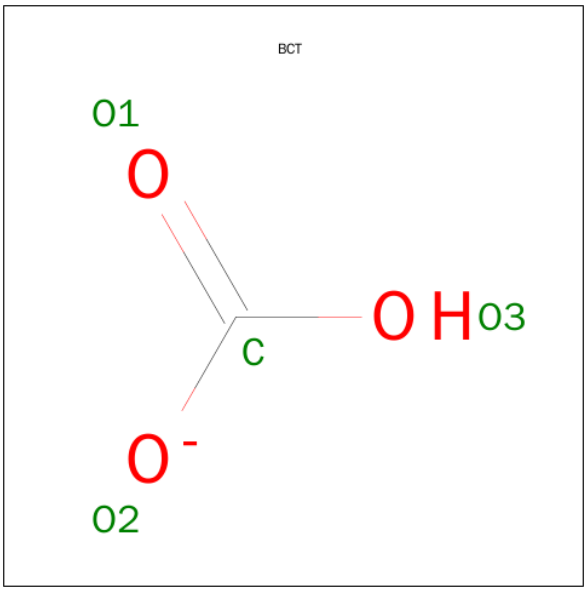
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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 4 1 3	0	0
5	B	1	Total C O 4 1 3	0	0
5	C	1	Total C O 4 1 3	0	0
5	D	1	Total C O 4 1 3	0	0
5	E	1	Total C O 4 1 3	0	0
5	F	1	Total C O 4 1 3	0	0

- Molecule 6 is water.

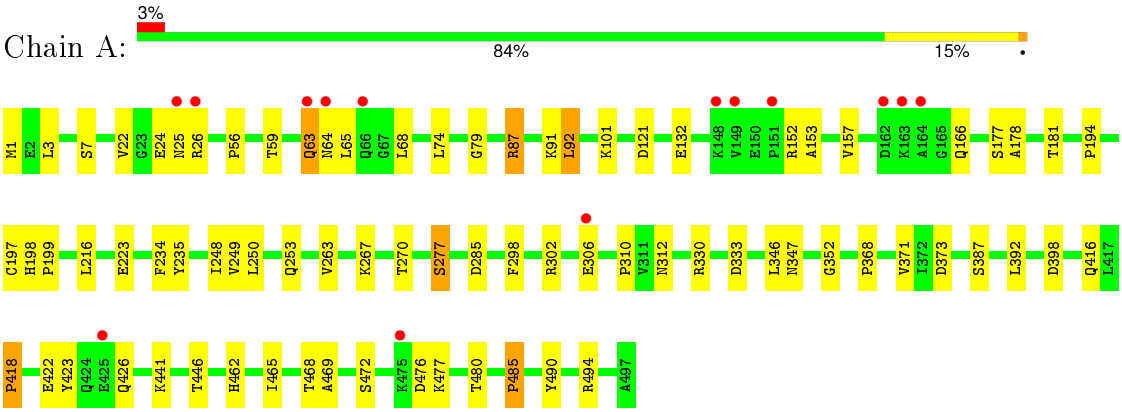
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	114	Total O 114 114	0	0
6	B	99	Total O 99 99	0	0
6	C	162	Total O 162 162	0	0
6	D	111	Total O 111 111	0	0
6	E	123	Total O 123 123	0	0
6	F	93	Total O 93 93	0	0

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.

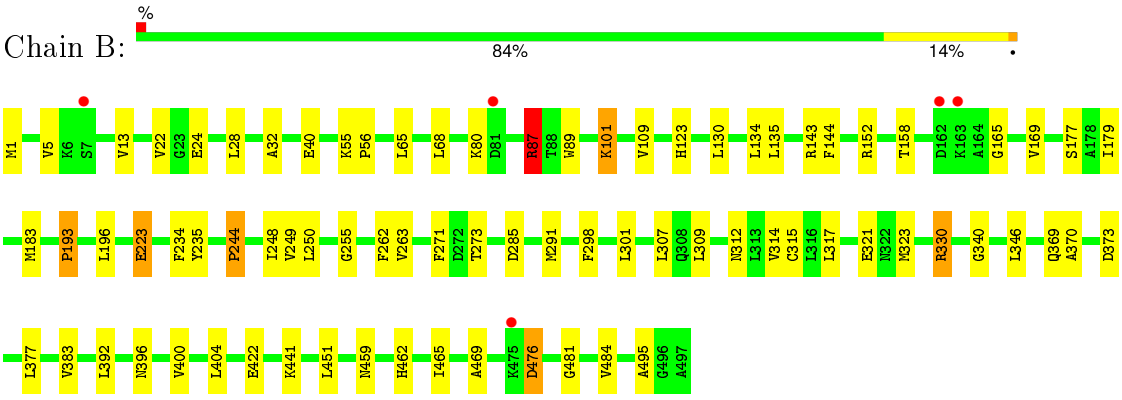
- Molecule 1: Cytosol aminopeptidase

Chain A:



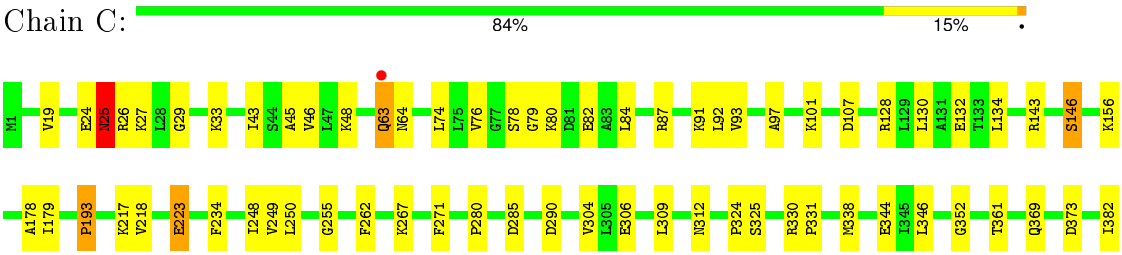
- Molecule 1: Cytosol aminopeptidase

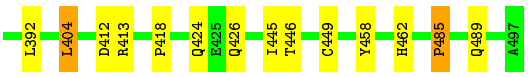
Chain B:



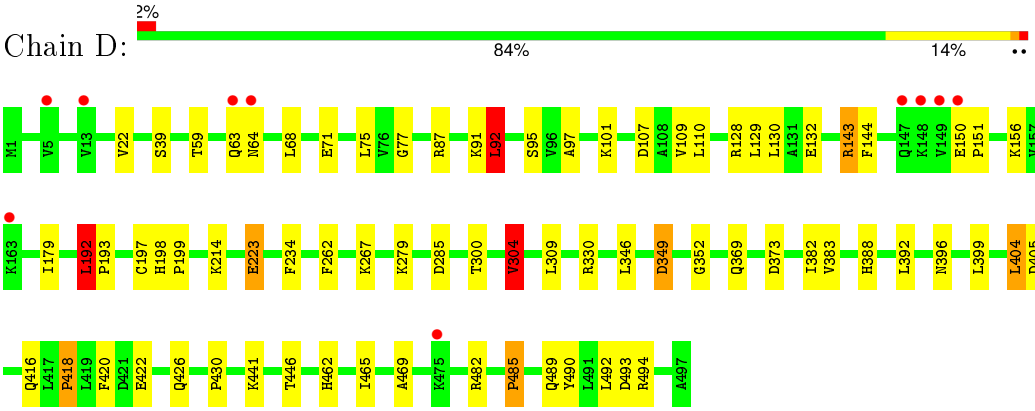
- Molecule 1: Cytosol aminopeptidase

Chain C:

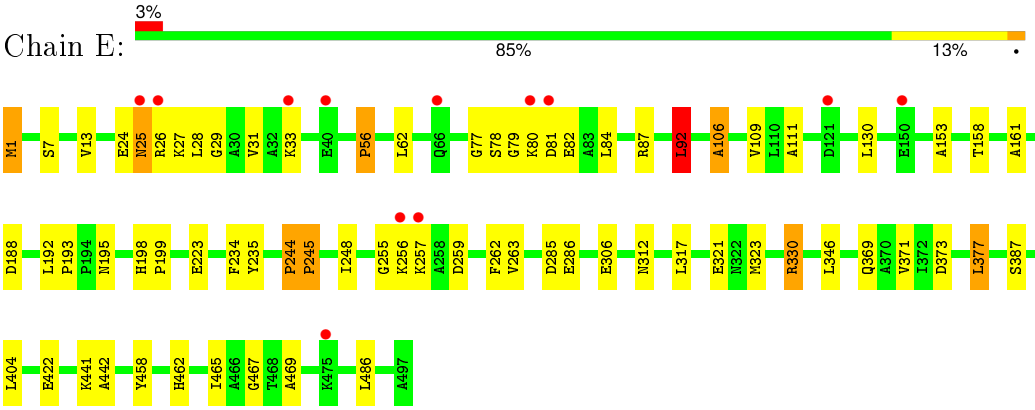




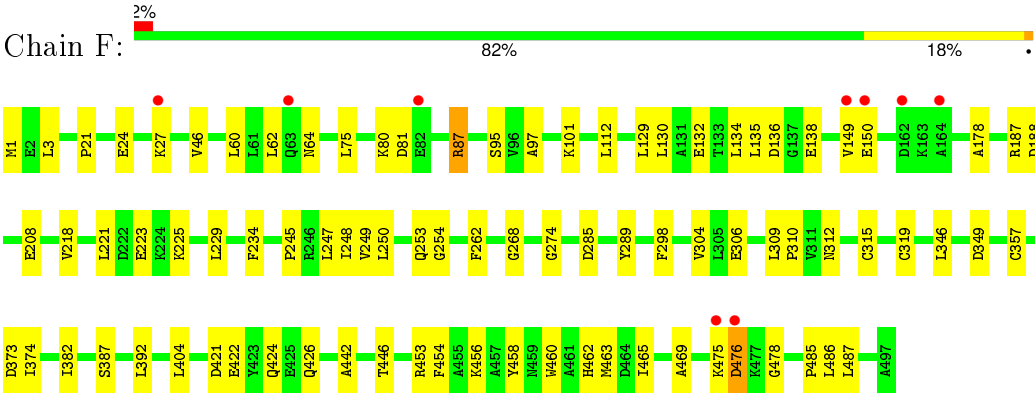
• Molecule 1: Cytosol aminopeptidase



• Molecule 1: Cytosol aminopeptidase



• Molecule 1: Cytosol aminopeptidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	95.79Å 95.93Å 96.31Å 68.43° 76.31° 94.86°	Depositor
Resolution (Å)	47.45 – 2.20 47.45 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (47.45-2.20) 74.3 (47.45-2.00)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.192 , 0.251 0.202 , 0.253	Depositor DCC
R_{free} test set	14341 reflections (11.02%)	DCC
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 166778 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	22836	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: BCT, 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	0.84	6/3737 (0.2%)	0.85	8/5054 (0.2%)
1	B	0.77	5/3737 (0.1%)	0.80	6/5054 (0.1%)
1	C	0.82	4/3737 (0.1%)	0.83	5/5054 (0.1%)
1	D	0.76	7/3737 (0.2%)	0.80	6/5054 (0.1%)
1	E	0.76	1/3737 (0.0%)	0.80	6/5054 (0.1%)
1	F	0.66	0/3737	0.71	1/5054 (0.0%)
All	All	0.77	23/22422 (0.1%)	0.80	32/30324 (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	A	0	1
1	C	0	2
1	D	0	1
1	E	0	2
All	All	0	6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	ASP	CB-CG	-7.52	1.35	1.51
1	A	418	PRO	N-CD	-7.33	1.37	1.47
1	B	223	GLU	CG-CD	7.22	1.62	1.51
1	D	430	PRO	N-CD	-6.98	1.38	1.47
1	C	82	GLU	CG-CD	-6.89	1.41	1.51
1	C	485	PRO	N-CD	-6.37	1.39	1.47
1	B	301	LEU	C-N	6.36	1.48	1.34
1	C	223	GLU	CG-CD	6.30	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	223	GLU	CG-CD	6.21	1.61	1.51
1	D	214	LYS	CB-CG	-6.17	1.35	1.52
1	B	193	PRO	N-CD	-6.09	1.39	1.47
1	A	22	VAL	CB-CG1	-5.94	1.40	1.52
1	C	193	PRO	N-CD	-5.83	1.39	1.47
1	E	245	PRO	N-CD	-5.48	1.40	1.47
1	D	418	PRO	N-CD	-5.45	1.40	1.47
1	A	485	PRO	N-CD	-5.39	1.40	1.47
1	B	40	GLU	C-N	-5.31	1.23	1.33
1	D	144	PHE	C-O	-5.29	1.13	1.23
1	B	22	VAL	CB-CG2	-5.26	1.41	1.52
1	A	310	PRO	N-CD	-5.25	1.40	1.47
1	D	304	VAL	CB-CG1	-5.23	1.41	1.52
1	A	423	TYR	CD2-CE2	-5.14	1.31	1.39
1	D	485	PRO	N-CD	-5.03	1.40	1.47

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	87	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	A	121	ASP	CB-CG-OD1	-10.20	109.12	118.30
1	E	245	PRO	CA-N-CD	-9.72	97.89	111.50
1	C	193	PRO	CA-N-CD	-9.56	98.12	111.50
1	B	193	PRO	CA-N-CD	-9.09	98.77	111.50
1	E	244	PRO	CA-N-CD	-9.04	98.85	111.50
1	D	485	PRO	CA-N-CD	-8.99	98.91	111.50
1	D	418	PRO	CA-N-CD	-8.99	98.92	111.50
1	A	310	PRO	CA-N-CD	-8.98	98.92	111.50
1	B	87	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	418	PRO	CA-N-CD	-8.77	99.22	111.50
1	B	244	PRO	CA-N-CD	-8.61	99.44	111.50
1	E	56	PRO	CA-N-CD	-8.52	99.57	111.50
1	C	485	PRO	CA-N-CD	-8.41	99.73	111.50
1	A	485	PRO	CA-N-CD	-8.39	99.75	111.50
1	C	280	PRO	C-N-CA	-8.38	104.71	122.30
1	D	430	PRO	CA-N-CD	-8.03	100.26	111.50
1	E	92	LEU	CA-CB-CG	7.71	133.04	115.30
1	B	330	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	A	1	MET	C-N-CA	7.16	139.59	121.70
1	D	92	LEU	CA-CB-CG	7.13	131.70	115.30
1	A	92	LEU	CA-CB-CG	6.57	130.41	115.30
1	D	349	ASP	CB-CG-OD1	6.33	124.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	192	LEU	CA-CB-CG	6.26	129.69	115.30
1	A	121	ASP	CB-CG-OD2	5.86	123.57	118.30
1	E	188	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	480	THR	C-N-CA	-5.80	110.13	122.30
1	B	301	LEU	O-C-N	-5.75	113.50	122.70
1	C	290	ASP	CB-CG-OD1	5.38	123.15	118.30
1	F	192	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	412	ASP	CB-CG-OD1	5.09	122.88	118.30
1	E	188	ASP	CB-CG-OD2	-5.04	113.76	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	GLN	Peptide
1	C	25	ASN	Peptide
1	C	63	GLN	Peptide
1	D	63	GLN	Peptide
1	E	106	ALA	Peptide
1	E	25	ASN	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	3682	0	3777	64	1
1	B	3682	0	3777	84	2
1	C	3682	0	3777	77	1
1	D	3682	0	3777	66	0
1	E	3682	0	3777	75	4
1	F	3682	0	3777	74	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	6	0
5	F	4	0	0	0	0
6	A	114	0	0	7	0
6	B	99	0	0	7	0
6	C	162	0	0	3	0
6	D	111	0	0	5	0
6	E	123	0	0	3	0
6	F	93	0	0	4	0
All	All	22836	0	22662	409	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (409) 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:F:101:LYS:HE3	1:F:138:GLU:OE2	1.28	1.33
1:F:27:LYS:HE2	1:F:81:ASP:OD1	1.30	1.31
1:C:223:GLU:HB3	6:C:3723:HOH:O	1.48	1.13
1:B:248:ILE:HG22	1:B:250:LEU:HD11	1.31	1.12
1:A:181:THR:HG21	1:A:306:GLU:OE2	1.51	1.10
1:D:39:SER:HB3	1:D:68:LEU:HD21	1.34	1.03
1:E:377:LEU:CD1	5:E:504:BCT:C	2.37	1.03
1:B:262:PHE:CZ	1:B:369:GLN:NE2	2.26	1.01
1:F:262:PHE:CZ	1:F:369:GLN:NE2	2.27	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:GLU:HB3	6:D:3693:HOH:O	1.61	1.00
1:C:262:PHE:CZ	1:C:369:GLN:NE2	2.29	1.00
1:D:39:SER:CB	1:D:68:LEU:HD21	1.92	0.99
1:F:101:LYS:CE	1:F:138:GLU:OE2	2.10	0.99
1:B:193:PRO:O	1:B:193:PRO:HD2	1.58	0.98
1:E:262:PHE:CZ	1:E:369:GLN:NE2	2.34	0.95
1:A:87:ARG:HA	1:A:87:ARG:HE	1.31	0.95
1:B:307:LEU:HB2	1:B:309:LEU:CD2	1.97	0.94
1:B:248:ILE:HG22	1:B:250:LEU:CD1	1.96	0.94
1:E:27:LYS:NZ	1:E:81:ASP:OD1	2.01	0.93
1:F:178:ALA:HA	1:F:306:GLU:OE1	1.68	0.93
1:F:188:ASP:O	1:F:192:LEU:HD23	1.66	0.93
1:B:373:ASP:OD1	1:B:462:HIS:HA	1.70	0.92
1:F:188:ASP:O	1:F:192:LEU:CD2	2.17	0.92
1:F:1:MET:HE2	1:F:135:LEU:HD23	1.52	0.92
1:E:377:LEU:HD12	5:E:504:BCT:O2	1.71	0.91
1:C:130:LEU:HD21	1:C:134:LEU:HD11	1.54	0.89
1:D:192:LEU:HG	1:D:197:CYS:HB2	1.53	0.89
1:A:181:THR:CG2	1:A:306:GLU:OE2	2.22	0.88
1:E:223:GLU:HB3	6:E:3720:HOH:O	1.75	0.87
1:F:248:ILE:HG22	1:F:250:LEU:HD11	1.57	0.87
1:B:248:ILE:CG2	1:B:250:LEU:HD11	2.05	0.86
1:F:1:MET:CE	1:F:135:LEU:HD23	2.07	0.85
1:B:307:LEU:CB	1:B:309:LEU:CD2	2.53	0.85
1:F:248:ILE:HG22	1:F:250:LEU:CD1	2.05	0.85
1:D:392:LEU:HD23	1:D:404:LEU:HD13	1.57	0.85
1:C:25:ASN:OD1	1:C:27:LYS:HD2	1.78	0.83
1:A:418:PRO:HD2	1:A:418:PRO:O	1.76	0.83
1:C:330:ARG:NH2	1:E:195:ASN:HA	1.94	0.82
1:A:178:ALA:HA	1:A:306:GLU:OE1	1.80	0.81
1:A:223:GLU:HB3	6:A:3688:HOH:O	1.80	0.81
1:C:193:PRO:HD2	1:C:193:PRO:O	1.81	0.80
1:D:373:ASP:OD1	1:D:462:HIS:HA	1.81	0.80
1:C:128:ARG:HH12	1:C:489:GLN:HE22	1.29	0.80
1:E:373:ASP:OD1	1:E:462:HIS:HA	1.80	0.80
1:E:377:LEU:CD1	5:E:504:BCT:O2	2.29	0.80
1:E:377:LEU:HD11	5:E:504:BCT:C	2.11	0.80
1:D:418:PRO:HD2	1:D:418:PRO:O	1.80	0.80
1:B:285:ASP:OD2	1:E:346:LEU:HD22	1.83	0.79
1:D:392:LEU:HD23	1:D:404:LEU:CD1	2.12	0.78
1:B:249:VAL:C	1:B:250:LEU:HD12	2.04	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:GLN:NE2	1:C:449:CYS:SG	2.58	0.77
1:C:248:ILE:HG22	1:C:250:LEU:CD1	2.13	0.77
1:D:300:THR:O	1:D:304:VAL:HG12	1.84	0.77
1:D:39:SER:CB	1:D:68:LEU:CD2	2.61	0.77
1:C:304:VAL:HG12	1:C:309:LEU:HD22	1.67	0.77
1:A:248:ILE:HG22	1:A:250:LEU:HD11	1.66	0.76
1:A:285:ASP:OD2	1:D:346:LEU:HD22	1.84	0.76
1:B:250:LEU:HD12	1:B:250:LEU:N	2.00	0.76
1:E:392:LEU:CD2	1:E:404:LEU:HD22	2.15	0.76
1:B:451:LEU:CD1	1:B:462:HIS:CD2	2.68	0.75
1:E:245:PRO:HD2	1:E:245:PRO:O	1.87	0.75
1:B:223:GLU:HB3	6:B:3698:HOH:O	1.86	0.75
1:E:56:PRO:HD3	1:E:79:GLY:CA	2.17	0.75
1:B:1:MET:HE2	1:B:135:LEU:HD23	1.69	0.74
1:B:244:PRO:O	1:B:244:PRO:HD2	1.86	0.74
1:C:25:ASN:HB2	1:C:27:LYS:HB2	1.70	0.74
1:A:373:ASP:OD1	1:A:462:HIS:HA	1.87	0.74
1:D:262:PHE:CZ	1:D:369:GLN:NE2	2.55	0.74
1:C:130:LEU:CD2	1:C:134:LEU:HD11	2.18	0.73
1:A:248:ILE:HG22	1:A:250:LEU:CD1	2.18	0.73
1:F:392:LEU:HD23	1:F:404:LEU:CD1	2.18	0.73
1:B:373:ASP:OD2	1:B:462:HIS:HD2	1.72	0.72
1:B:451:LEU:CD1	1:B:462:HIS:NE2	2.53	0.72
1:E:377:LEU:HD12	1:E:377:LEU:O	1.89	0.72
1:B:24:GLU:OE1	1:B:80:LYS:HG3	1.88	0.72
1:C:373:ASP:OD1	1:C:462:HIS:HA	1.89	0.72
1:C:267:LYS:HE3	1:C:352:GLY:HA3	1.71	0.72
1:F:27:LYS:HE2	1:F:81:ASP:CG	2.10	0.71
1:D:267:LYS:HE3	1:D:352:GLY:HA3	1.72	0.71
1:D:405:ASP:OD2	1:D:409:ARG:NH1	2.24	0.71
1:B:400:VAL:O	1:B:404:LEU:HD23	1.89	0.71
1:B:392:LEU:HD23	1:B:404:LEU:CD2	2.21	0.70
1:B:392:LEU:CD2	1:B:404:LEU:HD22	2.21	0.70
1:D:426:GLN:HE21	1:D:441:LYS:HE3	1.56	0.69
1:D:39:SER:HB3	1:D:68:LEU:CD2	2.19	0.69
1:B:373:ASP:OD2	1:B:462:HIS:CD2	2.46	0.69
1:B:87:ARG:HD2	1:F:422:GLU:OE2	1.92	0.69
1:E:109:VAL:HG22	1:E:158:THR:HB	1.73	0.69
1:C:217:LYS:HD2	1:C:218:VAL:N	2.07	0.69
1:A:249:VAL:C	1:A:250:LEU:HD12	2.13	0.69
1:B:451:LEU:HD12	1:B:462:HIS:CD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:373:ASP:OD1	1:F:462:HIS:HA	1.92	0.69
1:D:39:SER:HA	1:D:68:LEU:CD2	2.24	0.68
1:E:244:PRO:HD2	1:E:244:PRO:O	1.92	0.68
1:E:377:LEU:HD12	5:E:504:BCT:C	2.18	0.68
1:D:39:SER:CA	1:D:68:LEU:HD21	2.22	0.68
1:F:223:GLU:HB2	6:F:3716:HOH:O	1.92	0.68
1:D:267:LYS:HE3	1:D:352:GLY:CA	2.24	0.68
1:B:451:LEU:HD12	1:B:462:HIS:NE2	2.09	0.67
1:E:392:LEU:HD23	1:E:404:LEU:CD2	2.24	0.67
1:A:422:GLU:OE1	1:C:413:ARG:NH2	2.27	0.67
1:A:426:GLN:OE1	1:A:446:THR:HG21	1.94	0.67
1:B:307:LEU:CB	1:B:309:LEU:HD22	2.22	0.67
1:B:309:LEU:HD12	1:B:495:ALA:CB	2.24	0.67
1:D:285:ASP:OD2	1:F:346:LEU:HD22	1.95	0.67
1:F:188:ASP:O	1:F:192:LEU:HD22	1.95	0.67
1:C:25:ASN:O	1:C:26:ARG:HB2	1.94	0.67
1:A:87:ARG:HD3	1:A:91:LYS:HE3	1.77	0.66
1:C:267:LYS:HE3	1:C:352:GLY:CA	2.25	0.66
1:C:248:ILE:HG22	1:C:250:LEU:HD11	1.77	0.66
1:F:249:VAL:C	1:F:250:LEU:HD12	2.15	0.66
1:B:307:LEU:HB3	1:B:309:LEU:CD2	2.25	0.65
1:B:383:VAL:O	1:F:442:ALA:HA	1.97	0.65
1:B:193:PRO:O	1:B:193:PRO:CD	2.38	0.65
1:B:451:LEU:HD13	1:B:462:HIS:CD2	2.31	0.65
1:B:392:LEU:HD23	1:B:404:LEU:HD21	1.78	0.65
1:F:456:LYS:NZ	6:F:3247:HOH:O	2.21	0.65
1:D:128:ARG:HH12	1:D:489:GLN:HE22	1.45	0.65
1:B:250:LEU:CD1	1:B:250:LEU:N	2.59	0.65
1:D:192:LEU:HD12	1:D:193:PRO:HD2	1.78	0.65
1:C:330:ARG:HD3	1:E:321:GLU:OE2	1.97	0.64
1:A:472:SER:O	1:A:477:LYS:HD2	1.97	0.64
1:B:346:LEU:CD2	1:C:285:ASP:OD2	2.45	0.64
1:B:307:LEU:HB3	1:B:309:LEU:HD22	1.79	0.64
1:B:1:MET:CE	1:B:135:LEU:HD23	2.28	0.64
1:A:346:LEU:HD22	1:F:285:ASP:OD2	1.98	0.64
1:F:248:ILE:CG2	1:F:250:LEU:HD11	2.27	0.64
1:E:400:VAL:O	1:E:404:LEU:HD23	1.98	0.63
1:C:392:LEU:HD23	1:C:404:LEU:CD1	2.28	0.63
1:C:255:GLY:H	1:C:312:ASN:ND2	1.97	0.63
1:B:244:PRO:HD2	6:B:3694:HOH:O	1.99	0.62
1:C:178:ALA:HA	1:C:306:GLU:OE1	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:PRO:HD2	6:E:516:HOH:O	1.99	0.62
1:F:3:LEU:HD13	1:F:135:LEU:HD21	1.82	0.62
1:C:330:ARG:HH21	1:E:195:ASN:HA	1.65	0.62
1:A:426:GLN:OE1	1:A:446:THR:CG2	2.48	0.61
1:B:271:PHE:CD2	1:E:330:ARG:HG2	2.34	0.61
1:A:267:LYS:HE3	1:A:352:GLY:HA3	1.81	0.61
1:B:285:ASP:OD2	1:E:346:LEU:CD2	2.48	0.61
1:A:285:ASP:OD2	1:D:346:LEU:CD2	2.46	0.61
1:E:29:GLY:O	1:E:33:LYS:HG3	2.01	0.61
1:C:130:LEU:CD2	1:C:134:LEU:CD1	2.77	0.61
1:A:101:LYS:HD2	1:A:152:ARG:NE	2.15	0.61
1:C:97:ALA:O	1:C:101:LYS:HG3	2.00	0.61
1:D:39:SER:CA	1:D:68:LEU:CD2	2.78	0.61
1:B:307:LEU:HB2	1:B:309:LEU:HD23	1.81	0.60
1:B:307:LEU:CB	1:B:309:LEU:HD21	2.31	0.60
1:D:426:GLN:NE2	1:D:441:LYS:HE3	2.17	0.60
1:E:56:PRO:HD3	1:E:79:GLY:N	2.16	0.60
1:C:43:ILE:O	1:C:46:VAL:HG22	2.01	0.60
1:E:24:GLU:C	1:E:26:ARG:H	2.05	0.60
1:E:25:ASN:HB3	1:E:27:LYS:HB2	1.84	0.60
1:C:76:VAL:HG22	1:C:92:LEU:CD2	2.32	0.59
1:D:409:ARG:NH2	1:D:493:ASP:OD2	2.36	0.59
1:E:387:SER:HA	1:E:467:GLY:O	2.02	0.59
1:C:130:LEU:O	1:C:134:LEU:HG	2.02	0.59
1:C:223:GLU:CB	6:C:3723:HOH:O	2.26	0.59
1:A:418:PRO:CD	1:A:418:PRO:O	2.51	0.59
1:B:392:LEU:CD2	1:B:404:LEU:CD2	2.79	0.59
1:B:370:ALA:HB2	6:B:3777:HOH:O	2.02	0.59
1:D:426:GLN:OE1	1:D:446:THR:HG21	2.03	0.58
1:C:130:LEU:HD21	1:C:134:LEU:CD1	2.32	0.58
1:C:128:ARG:HH12	1:C:489:GLN:NE2	1.99	0.58
1:E:392:LEU:HD23	1:E:404:LEU:HD22	1.82	0.58
1:D:441:LYS:HG2	6:D:3713:HOH:O	2.03	0.58
1:F:253:GLN:HA	1:F:312:ASN:HD22	1.69	0.58
1:D:223:GLU:CB	6:D:3693:HOH:O	2.36	0.56
1:D:22:VAL:O	1:D:77:GLY:HA2	2.05	0.56
1:E:56:PRO:HD3	1:E:79:GLY:HA3	1.88	0.56
1:F:424:GLN:HE21	1:F:453:ARG:HH21	1.53	0.56
1:A:64:ASN:O	1:A:64:ASN:OD1	2.24	0.56
1:F:426:GLN:OE1	1:F:446:THR:HG21	2.06	0.56
1:A:330:ARG:NH1	1:A:333:ASP:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:LYS:HD2	1:C:218:VAL:H	1.70	0.55
1:B:101:LYS:HD2	1:B:152:ARG:HH12	1.69	0.55
1:E:255:GLY:H	1:E:312:ASN:ND2	2.05	0.55
1:C:424:GLN:NE2	1:C:449:CYS:CB	2.70	0.55
1:A:277:SER:CB	1:A:347:ASN:OD1	2.55	0.55
1:A:3:LEU:CD2	1:A:157:VAL:HB	2.37	0.55
1:C:424:GLN:HE22	1:C:449:CYS:CB	2.20	0.55
1:A:346:LEU:CD2	1:F:285:ASP:OD2	2.54	0.55
1:B:1:MET:CE	1:B:134:LEU:HG	2.36	0.55
1:B:250:LEU:HB2	1:B:315:CYS:HB2	1.89	0.55
1:E:462:HIS:HE1	6:E:550:HOH:O	1.89	0.55
1:A:223:GLU:HG2	1:A:235:TYR:HE1	1.72	0.55
1:E:56:PRO:CD	1:E:79:GLY:CA	2.83	0.54
1:B:101:LYS:HG2	1:B:152:ARG:NH1	2.22	0.54
1:F:465:ILE:HD12	1:F:469:ALA:HB2	1.88	0.54
1:C:248:ILE:CG2	1:C:250:LEU:HD11	2.36	0.54
1:A:25:ASN:O	1:A:26:ARG:HB2	2.06	0.54
1:B:263:VAL:HG22	1:B:314:VAL:HB	1.88	0.54
1:E:285:ASP:OD1	1:E:286:GLU:N	2.41	0.54
1:C:76:VAL:CG2	1:C:92:LEU:CD2	2.85	0.54
1:D:87:ARG:HG3	1:D:91:LYS:HE2	1.90	0.54
1:D:279:LYS:HE2	1:D:349:ASP:OD1	2.07	0.54
1:B:144:PHE:HZ	1:B:196:LEU:HD12	1.73	0.54
1:E:223:GLU:OE1	1:E:244:PRO:HB3	2.08	0.53
1:C:330:ARG:HH21	1:E:195:ASN:CA	2.20	0.53
1:A:248:ILE:CG2	1:A:250:LEU:HD11	2.34	0.53
1:D:418:PRO:CD	1:D:418:PRO:O	2.55	0.53
1:F:387:SER:HB3	6:F:865:HOH:O	2.08	0.53
1:C:338:MET:HE2	1:C:361:THR:HB	1.90	0.53
1:B:89:TRP:CZ2	1:B:130:LEU:HD12	2.43	0.53
1:E:377:LEU:HD11	5:E:504:BCT:O1	2.08	0.53
1:A:267:LYS:HE3	1:A:352:GLY:CA	2.39	0.53
1:F:132:GLU:OE2	1:F:485:PRO:HG3	2.09	0.52
1:E:28:LEU:O	1:E:33:LYS:HD2	2.08	0.52
1:D:426:GLN:OE1	1:D:446:THR:CG2	2.57	0.52
1:D:465:ILE:HD12	1:D:469:ALA:HB2	1.92	0.52
1:E:223:GLU:HB2	1:E:245:PRO:HD2	1.92	0.52
1:C:193:PRO:CD	1:C:193:PRO:O	2.56	0.52
1:C:130:LEU:HD23	1:C:134:LEU:CD1	2.40	0.52
1:F:475:LYS:HG3	1:F:476:ASP:OD1	2.09	0.52
1:F:1:MET:HE3	1:F:135:LEU:HD23	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:GLN:OE1	1:C:446:THR:HG21	2.10	0.51
1:E:77:GLY:O	1:E:92:LEU:HD22	2.09	0.51
1:C:392:LEU:HD23	1:C:404:LEU:HD13	1.90	0.51
1:A:63:GLN:OE1	1:E:62:LEU:CD2	2.58	0.51
1:E:7:SER:HA	1:E:161:ALA:O	2.11	0.51
1:B:400:VAL:HG12	1:B:404:LEU:HD23	1.93	0.51
1:B:346:LEU:HD23	1:C:285:ASP:OD2	2.10	0.51
1:E:392:LEU:CD2	1:E:404:LEU:CD2	2.83	0.51
1:B:101:LYS:HD2	1:B:152:ARG:NH1	2.26	0.51
1:F:223:GLU:HG3	1:F:245:PRO:HD2	1.92	0.51
1:C:218:VAL:HG22	1:C:250:LEU:HG	1.91	0.51
1:B:244:PRO:CD	6:B:3694:HOH:O	2.56	0.50
1:A:59:THR:HB	1:A:74:LEU:HD11	1.93	0.50
1:D:198:HIS:HB2	1:D:199:PRO:CD	2.41	0.50
1:D:109:VAL:HG22	1:D:158:THR:HB	1.93	0.50
1:E:223:GLU:HB2	1:E:245:PRO:CD	2.42	0.49
1:F:250:LEU:HB2	1:F:315:CYS:HB2	1.93	0.49
1:A:462:HIS:HE1	6:A:538:HOH:O	1.95	0.49
1:D:382:ILE:HG22	1:E:441:LYS:HG2	1.92	0.49
1:B:244:PRO:CD	1:B:244:PRO:O	2.58	0.49
1:A:87:ARG:NE	1:A:87:ARG:HA	2.13	0.49
1:D:396:ASN:HD22	1:D:399:LEU:H	1.60	0.49
1:E:245:PRO:CD	1:E:245:PRO:O	2.59	0.49
1:C:76:VAL:HG21	1:C:92:LEU:HD22	1.95	0.49
1:F:424:GLN:NE2	1:F:453:ARG:HE	2.10	0.49
1:A:7:SER:HB2	1:A:166:GLN:OE1	2.13	0.49
1:F:27:LYS:CE	1:F:81:ASP:OD1	2.26	0.49
1:D:132:GLU:OE2	1:D:485:PRO:HG3	2.13	0.49
1:C:130:LEU:HD23	1:C:134:LEU:HD12	1.95	0.49
1:C:249:VAL:C	1:C:250:LEU:HD12	2.33	0.49
1:E:178:ALA:HA	1:E:306:GLU:OE1	2.12	0.49
1:A:223:GLU:CB	6:A:3688:HOH:O	2.52	0.48
1:B:255:GLY:HA2	6:B:3748:HOH:O	2.13	0.48
1:B:255:GLY:H	1:B:312:ASN:ND2	2.11	0.48
1:F:97:ALA:HB1	1:F:101:LYS:NZ	2.28	0.48
1:C:179:ILE:HG23	1:C:485:PRO:HD3	1.95	0.48
1:F:426:GLN:OE1	1:F:446:THR:CG2	2.60	0.48
1:E:1:MET:HB2	1:E:1:MET:HE2	1.67	0.48
1:D:373:ASP:OD1	1:D:462:HIS:CA	2.58	0.48
1:F:21:PRO:HD3	1:F:112:LEU:HD23	1.94	0.48
1:D:143:ARG:HB3	6:D:3730:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:PRO:O	1:E:244:PRO:CD	2.62	0.48
1:C:330:ARG:O	1:C:331:PRO:C	2.52	0.48
1:A:101:LYS:HD2	1:A:152:ARG:HE	1.78	0.48
1:A:177:SER:HB3	6:A:760:HOH:O	2.12	0.48
1:F:149:VAL:HG12	1:F:150:GLU:O	2.13	0.48
1:D:392:LEU:CD2	1:D:404:LEU:HD13	2.36	0.47
1:C:424:GLN:NE2	1:C:449:CYS:HB3	2.28	0.47
1:A:132:GLU:OE2	1:A:485:PRO:HG3	2.14	0.47
1:A:250:LEU:N	1:A:250:LEU:HD12	2.29	0.47
1:C:330:ARG:HH22	1:E:195:ASN:HA	1.74	0.47
1:E:373:ASP:OD1	1:E:462:HIS:CA	2.58	0.47
1:E:392:LEU:HD23	1:E:404:LEU:HD21	1.93	0.47
1:E:56:PRO:CD	1:E:79:GLY:HA3	2.44	0.47
1:B:321:GLU:HG2	1:B:323:MET:HG2	1.95	0.47
1:E:321:GLU:HG2	1:E:323:MET:HG2	1.96	0.47
1:A:263:VAL:HG23	1:A:368:PRO:HB3	1.96	0.47
1:E:130:LEU:C	1:E:130:LEU:HD23	2.35	0.47
1:F:250:LEU:HD12	1:F:250:LEU:N	2.28	0.47
1:A:277:SER:HB3	1:A:347:ASN:OD1	2.15	0.47
1:F:218:VAL:HG22	1:F:250:LEU:HG	1.97	0.47
1:A:24:GLU:O	1:A:25:ASN:CB	2.62	0.47
1:F:486:LEU:HD23	1:F:486:LEU:C	2.36	0.46
1:F:374:ILE:N	1:F:374:ILE:HD12	2.30	0.46
1:C:324:PRO:O	1:C:325:SER:HB3	2.15	0.46
1:F:262:PHE:HZ	1:F:369:GLN:NE2	2.06	0.46
1:D:396:ASN:ND2	1:D:399:LEU:H	2.14	0.46
1:A:253:GLN:HA	1:A:312:ASN:HD22	1.80	0.46
1:C:45:ALA:HA	1:C:48:LYS:HD2	1.97	0.46
1:D:97:ALA:O	1:D:101:LYS:HG3	2.16	0.46
1:F:392:LEU:HD13	1:F:463:MET:HG2	1.97	0.46
1:A:24:GLU:O	1:A:25:ASN:HB2	2.16	0.46
1:C:24:GLU:HG3	1:C:79:GLY:C	2.36	0.46
1:D:179:ILE:CG2	1:D:485:PRO:HD3	2.45	0.46
1:F:136:ASP:OD1	1:F:187:ARG:NH1	2.48	0.46
1:B:262:PHE:CE2	1:B:369:GLN:NE2	2.81	0.46
1:D:392:LEU:O	1:D:416:GLN:HA	2.16	0.46
1:D:462:HIS:HE1	6:D:528:HOH:O	1.98	0.45
1:E:106:ALA:HA	1:E:153:ALA:O	2.17	0.45
1:E:465:ILE:HD12	1:E:469:ALA:HB2	1.98	0.45
1:E:198:HIS:HB2	1:E:199:PRO:CD	2.47	0.45
1:F:374:ILE:HG12	1:F:487:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:SER:O	1:C:84:LEU:HD21	2.16	0.45
1:F:262:PHE:CE2	1:F:369:GLN:NE2	2.82	0.45
1:D:412:ASP:OD1	1:D:482:ARG:NE	2.47	0.45
1:F:460:TRP:CZ2	1:F:462:HIS:HB2	2.52	0.45
1:F:130:LEU:HD23	1:F:130:LEU:C	2.37	0.45
1:E:248:ILE:HB	1:E:317:LEU:HB2	1.99	0.44
1:D:128:ARG:HH22	1:D:489:GLN:NE2	2.15	0.44
1:D:77:GLY:O	1:D:92:LEU:HD22	2.18	0.44
1:B:5:VAL:HG21	1:B:169:VAL:HG12	1.98	0.44
1:B:441:LYS:HG2	1:F:382:ILE:HG22	1.99	0.44
1:E:78:SER:O	1:E:84:LEU:HD21	2.17	0.44
1:A:490:TYR:O	1:A:494:ARG:HG2	2.16	0.44
1:A:465:ILE:HD12	1:A:469:ALA:HB2	1.99	0.44
1:F:250:LEU:N	1:F:250:LEU:CD1	2.81	0.44
1:C:250:LEU:N	1:C:250:LEU:HD12	2.32	0.44
1:A:302:ARG:HG3	6:A:3785:HOH:O	2.16	0.44
1:A:65:LEU:HB2	1:A:68:LEU:HD12	1.99	0.44
1:F:221:LEU:HD22	1:F:247:LEU:HD23	1.99	0.44
1:B:330:ARG:HG2	1:C:271:PHE:CD2	2.53	0.44
1:B:271:PHE:HE2	1:B:273:THR:HG22	1.83	0.44
1:E:223:GLU:HG2	1:E:235:TYR:HE1	1.83	0.44
1:B:404:LEU:HD12	6:B:535:HOH:O	2.17	0.44
1:F:24:GLU:OE1	1:F:80:LYS:HG3	2.17	0.44
1:E:80:LYS:O	1:E:82:GLU:N	2.51	0.44
1:B:465:ILE:HD12	1:B:469:ALA:HB2	1.98	0.43
1:D:383:VAL:O	1:E:442:ALA:HA	2.19	0.43
1:A:3:LEU:HD23	1:A:157:VAL:HB	1.98	0.43
1:C:91:LYS:HG3	6:C:3783:HOH:O	2.17	0.43
1:C:63:GLN:O	1:C:64:ASN:O	2.36	0.43
1:E:263:VAL:HB	1:E:371:VAL:HG22	2.00	0.43
1:F:188:ASP:C	1:F:192:LEU:HD23	2.35	0.43
1:E:257:LYS:HD2	1:E:257:LYS:HA	1.66	0.43
1:B:476:ASP:N	1:B:476:ASP:OD1	2.51	0.43
1:C:25:ASN:OD1	1:C:27:LYS:HB2	2.17	0.43
1:A:216:LEU:HD11	1:A:250:LEU:HB3	1.99	0.43
1:B:143:ARG:HB2	6:B:513:HOH:O	2.19	0.43
1:B:441:LYS:HG2	1:F:382:ILE:CG2	2.49	0.43
1:B:109:VAL:HG22	1:B:158:THR:HB	2.00	0.43
1:A:198:HIS:HB2	1:A:199:PRO:CD	2.48	0.43
1:F:268:GLY:O	1:F:319:CYS:HA	2.19	0.43
1:F:367:LYS:N	1:F:368:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LEU:O	1:A:416:GLN:HA	2.18	0.43
1:A:153:ALA:HA	6:A:3779:HOH:O	2.19	0.43
1:E:192:LEU:HD23	1:E:193:PRO:HD2	2.00	0.43
1:C:29:GLY:O	1:C:33:LYS:HG3	2.18	0.43
1:C:330:ARG:HH21	1:E:195:ASN:N	2.16	0.43
1:D:64:ASN:HB3	1:D:71:GLU:O	2.18	0.43
1:B:223:GLU:HG2	1:B:235:TYR:HE1	1.84	0.42
1:D:128:ARG:HH12	1:D:489:GLN:NE2	2.14	0.42
1:F:204:GLU:O	1:F:208:GLU:HG3	2.19	0.42
1:A:387:SER:O	1:A:468:THR:HG22	2.19	0.42
1:B:346:LEU:HD22	1:C:285:ASP:OD2	2.17	0.42
1:A:253:GLN:HA	1:A:312:ASN:ND2	2.35	0.42
1:F:392:LEU:HD23	1:F:404:LEU:HD12	2.00	0.42
1:C:392:LEU:CD2	1:C:404:LEU:HD13	2.48	0.42
1:B:144:PHE:CZ	1:B:196:LEU:HD12	2.52	0.42
1:C:426:GLN:OE1	1:C:446:THR:CG2	2.67	0.42
1:B:396:ASN:HD22	1:B:459:ASN:HB3	1.84	0.42
1:C:132:GLU:OE2	1:C:485:PRO:HG3	2.19	0.42
1:F:424:GLN:HE22	1:F:453:ARG:HE	1.67	0.42
1:F:274:GLY:HA2	1:F:349:ASP:OD1	2.20	0.42
1:D:490:TYR:O	1:D:494:ARG:HG2	2.20	0.42
1:A:250:LEU:N	1:A:250:LEU:CD1	2.83	0.42
1:A:87:ARG:CA	1:A:87:ARG:HE	1.96	0.42
1:B:179:ILE:O	1:B:183:MET:HG3	2.20	0.42
1:F:1:MET:CE	1:F:134:LEU:HG	2.49	0.42
1:C:330:ARG:NH2	1:E:195:ASN:CA	2.71	0.42
1:C:392:LEU:CD2	1:C:404:LEU:CD1	2.96	0.42
1:E:29:GLY:O	1:E:33:LYS:CG	2.68	0.42
1:D:110:LEU:HB2	1:D:159:LEU:HD23	2.02	0.42
1:A:197:CYS:O	1:A:270:THR:HB	2.19	0.41
1:F:254:GLY:O	1:F:310:PRO:HA	2.19	0.41
1:F:225:LYS:NZ	1:F:229:LEU:HD21	2.35	0.41
1:E:486:LEU:HD23	1:E:486:LEU:C	2.39	0.41
1:A:441:LYS:HG2	1:C:382:ILE:HG23	2.02	0.41
1:F:60:LEU:HD22	1:F:75:LEU:HD12	2.02	0.41
1:F:46:VAL:HG11	1:F:62:LEU:HD21	2.03	0.41
1:D:150:GLU:HA	1:D:151:PRO:HD3	1.87	0.41
1:B:481:GLY:O	1:B:484:VAL:HG23	2.20	0.41
1:D:420:PHE:HB3	1:D:422:GLU:OE1	2.20	0.41
1:E:262:PHE:HZ	1:E:369:GLN:NE2	2.10	0.41
1:A:263:VAL:HB	1:A:371:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LYS:O	1:B:56:PRO:C	2.59	0.41
1:B:248:ILE:HB	1:B:317:LEU:HB2	2.03	0.41
1:B:377:LEU:HD22	1:B:462:HIS:CE1	2.56	0.41
1:B:330:ARG:HD2	1:B:330:ARG:HH11	1.63	0.41
1:F:304:VAL:HG13	1:F:309:LEU:HB2	2.01	0.41
1:B:422:GLU:OE2	1:F:87:ARG:NH1	2.49	0.41
1:F:46:VAL:HG23	6:F:1725:HOH:O	2.21	0.41
1:C:19:VAL:HG22	1:C:74:LEU:HB3	2.02	0.41
1:B:28:LEU:HD22	1:B:32:ALA:HB1	2.02	0.41
1:E:31:VAL:HG11	1:E:111:ALA:HB1	2.03	0.41
1:C:93:VAL:HG13	1:C:134:LEU:HD21	2.03	0.41
1:D:128:ARG:NH1	1:D:489:GLN:HE22	2.16	0.41
1:A:56:PRO:HD3	1:A:79:GLY:HA3	2.03	0.41
1:D:388:HIS:CE1	1:E:422:GLU:HB3	2.56	0.41
1:C:25:ASN:CB	1:C:27:LYS:HB2	2.47	0.41
1:D:198:HIS:HB2	1:D:199:PRO:HD2	2.01	0.41
1:F:289:TYR:OH	1:F:478:GLY:HA2	2.20	0.41
1:C:107:ASP:HA	1:C:156:LYS:O	2.21	0.41
1:A:476:ASP:HB2	6:A:3746:HOH:O	2.20	0.40
1:D:107:ASP:HA	1:D:156:LYS:O	2.22	0.40
1:D:309:LEU:HD21	1:D:492:LEU:HD23	2.03	0.40
1:E:28:LEU:HB2	1:E:33:LYS:HG2	2.02	0.40
1:D:59:THR:HA	1:D:75:LEU:O	2.21	0.40
1:A:194:PRO:HB2	1:D:330:ARG:HD2	2.03	0.40
1:F:357:CYS:HB2	1:F:454:PHE:CD1	2.57	0.40
1:B:400:VAL:CG1	1:B:404:LEU:HD23	2.51	0.40
1:C:418:PRO:HD2	1:C:445:ILE:HD11	2.04	0.40
1:B:65:LEU:HB2	1:B:68:LEU:HD12	2.04	0.40
1:C:344:GLU:HG2	1:C:346:LEU:HD12	2.03	0.40
1:D:130:LEU:C	1:D:130:LEU:HD23	2.41	0.40
1:B:123:HIS:CE1	1:B:165:GLY:HA3	2.56	0.40

All (4) 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:A:398:ASP:OD2	1:E:256:LYS:CE[1_455]	1.66	0.54
1:C:146:SER:O	1:E:26:ARG:NH2[1_554]	1.77	0.43
1:B:340:GLY:CA	1:E:25:ASN:ND2[1_554]	2.12	0.08
1:B:340:GLY:C	1:E:25:ASN:ND2[1_554]	2.18	0.02

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	495/497 (100%)	478 (97%)	17 (3%)	0	100	100
1	B	495/497 (100%)	475 (96%)	20 (4%)	0	100	100
1	C	495/497 (100%)	478 (97%)	16 (3%)	1 (0%)	52	59
1	D	495/497 (100%)	478 (97%)	17 (3%)	0	100	100
1	E	495/497 (100%)	475 (96%)	20 (4%)	0	100	100
1	F	495/497 (100%)	479 (97%)	15 (3%)	1 (0%)	52	59
All	All	2970/2982 (100%)	2863 (96%)	105 (4%)	2 (0%)	56	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	64	ASN
1	C	25	ASN

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	378/378 (100%)	373 (99%)	5 (1%)	76	87
1	B	378/378 (100%)	370 (98%)	8 (2%)	61	74
1	C	378/378 (100%)	371 (98%)	7 (2%)	65	77
1	D	378/378 (100%)	370 (98%)	8 (2%)	61	74
1	E	378/378 (100%)	369 (98%)	9 (2%)	57	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	378/378 (100%)	370 (98%)	8 (2%)	61 74
All	All	2268/2268 (100%)	2223 (98%)	45 (2%)	63 76

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ARG
1	A	92	LEU
1	A	234	PHE
1	A	277	SER
1	A	298	PHE
1	B	13	VAL
1	B	87	ARG
1	B	101	LYS
1	B	177	SER
1	B	234	PHE
1	B	291	MET
1	B	298	PHE
1	B	476	ASP
1	C	80	LYS
1	C	87	ARG
1	C	143	ARG
1	C	146	SER
1	C	234	PHE
1	C	404	LEU
1	C	458	TYR
1	D	92	LEU
1	D	95	SER
1	D	129	LEU
1	D	143	ARG
1	D	192	LEU
1	D	234	PHE
1	D	304	VAL
1	D	404	LEU
1	E	1	MET
1	E	13	VAL
1	E	87	ARG
1	E	92	LEU
1	E	234	PHE
1	E	259	ASP
1	E	330	ARG
1	E	377	LEU

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Mol	Chain	Res	Type
1	E	458	TYR
1	F	87	ARG
1	F	95	SER
1	F	129	LEU
1	F	234	PHE
1	F	298	PHE
1	F	421	ASP
1	F	458	TYR
1	F	476	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	312	ASN
1	A	459	ASN
1	A	462	HIS
1	B	312	ASN
1	B	462	HIS
1	C	123	HIS
1	C	312	ASN
1	C	424	GLN
1	C	489	GLN
1	D	312	ASN
1	D	388	HIS
1	D	396	ASN
1	D	426	GLN
1	D	459	ASN
1	D	462	HIS
1	D	489	GLN
1	E	312	ASN
1	E	462	HIS
1	F	312	ASN
1	F	424	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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 24 ligands modelled in this entry, 18 are monoatomic - leaving 6 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	-
5	BCT	B	504	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	C	504	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	D	504	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	E	504	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	F	504	-	0,3,3	0.00	-	0,3,3	0.00	-

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
5	BCT	B	504	-	-	0/0/0/0	0/0/0/0
5	BCT	C	504	-	-	0/0/0/0	0/0/0/0
5	BCT	D	504	-	-	0/0/0/0	0/0/0/0
5	BCT	E	504	-	-	0/0/0/0	0/0/0/0
5	BCT	F	504	-	-	0/0/0/0	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 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	504	BCT	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	497/497 (100%)	-0.33	14 (2%)	56	55	2, 11, 27, 41	0
1	B	497/497 (100%)	-0.25	5 (1%)	84	83	3, 15, 28, 41	0
1	C	497/497 (100%)	-0.38	1 (0%)	95	95	2, 9, 23, 35	0
1	D	497/497 (100%)	-0.27	11 (2%)	65	64	4, 13, 28, 51	0
1	E	497/497 (100%)	-0.25	13 (2%)	59	58	2, 12, 30, 43	0
1	F	497/497 (100%)	-0.23	9 (1%)	71	70	3, 13, 26, 38	0
All	All	2982/2982 (100%)	-0.29	53 (1%)	71	70	2, 12, 27, 51	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	25	ASN	7.1
1	D	149	VAL	6.3
1	D	148	LYS	5.8
1	D	147	GLN	4.9
1	E	81	ASP	4.5
1	A	63	GLN	4.3
1	D	63	GLN	4.1
1	B	475	LYS	3.8
1	F	63	GLN	3.8
1	F	164	ALA	3.8
1	A	148	LYS	3.8
1	D	150	GLU	3.7
1	F	82	GLU	3.6
1	C	63	GLN	3.5
1	E	80	LYS	3.5
1	A	306	GLU	3.4
1	F	149	VAL	3.3
1	A	26	ARG	3.1
1	D	475	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	163	LYS	2.8
1	A	64	ASN	2.7
1	A	163	LYS	2.7
1	D	64	ASN	2.7
1	B	162	ASP	2.6
1	A	162	ASP	2.6
1	A	151	PRO	2.6
1	D	5	VAL	2.5
1	E	66	GLN	2.5
1	E	475	LYS	2.5
1	B	7	SER	2.5
1	F	475	LYS	2.4
1	B	81	ASP	2.4
1	E	257	LYS	2.3
1	A	66	GLN	2.3
1	D	162	ASP	2.3
1	E	164	ALA	2.3
1	A	425	GLU	2.3
1	A	164	ALA	2.2
1	D	163	LYS	2.2
1	E	121	ASP	2.2
1	E	26	ARG	2.1
1	A	149	VAL	2.1
1	E	40	GLU	2.1
1	F	162	ASP	2.1
1	A	475	LYS	2.1
1	A	25	ASN	2.1
1	F	476	ASP	2.1
1	E	33	LYS	2.1
1	E	256	LYS	2.1
1	F	150	GLU	2.0
1	D	13	VAL	2.0
1	E	150	GLU	2.0
1	F	27	LYS	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	MN	F	502	1/1	0.98	0.13	1.02	37,37,37,37	0
3	MN	C	502	1/1	0.89	0.11	0.11	34,34,34,34	0
5	BCT	F	504	4/4	0.97	0.12	0.07	11,11,12,13	0
5	BCT	A	504	4/4	0.97	0.10	-0.29	10,11,12,14	0
5	BCT	B	504	4/4	0.98	0.10	-0.76	12,12,13,13	0
5	BCT	E	504	4/4	0.98	0.10	-0.89	7,7,8,9	0
5	BCT	C	504	4/4	0.99	0.08	-1.31	7,9,9,9	0
4	K	C	503	1/1	1.00	0.10	-1.36	12,12,12,12	0
3	MN	D	502	1/1	0.97	0.09	-1.43	35,35,35,35	0
4	K	B	503	1/1	0.98	0.09	-1.53	13,13,13,13	0
4	K	D	503	1/1	0.99	0.06	-1.91	10,10,10,10	0
4	K	F	503	1/1	0.98	0.08	-2.06	21,21,21,21	0
3	MN	B	502	1/1	0.96	0.08	-2.51	34,34,34,34	0
5	BCT	D	504	4/4	0.98	0.07	-2.64	11,12,12,13	0
4	K	A	503	1/1	0.99	0.07	-2.81	9,9,9,9	0
4	K	E	503	1/1	1.00	0.07	-3.06	12,12,12,12	0
2	ZN	D	501	1/1	1.00	0.05	-3.67	21,21,21,21	0
2	ZN	E	501	1/1	1.00	0.06	-3.68	18,18,18,18	0
3	MN	A	502	1/1	0.97	0.07	-3.85	37,37,37,37	0
2	ZN	F	501	1/1	0.98	0.05	-4.04	20,20,20,20	0
2	ZN	A	501	1/1	0.99	0.03	-4.22	20,20,20,20	0
3	MN	E	502	1/1	0.97	0.07	-4.37	33,33,33,33	0
2	ZN	C	501	1/1	0.99	0.03	-5.16	17,17,17,17	0
2	ZN	B	501	1/1	1.00	0.04	-5.44	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.