Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 11:18 AM EDT

PDB ID	:	5BZA
Title	:	Crystal structure of CbsA from Thermotoga neapolitana
Authors	:	Ha, N.C.; Kim, J.S.; Yoon, B.Y.
Deposited on	:	2015-06-11
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

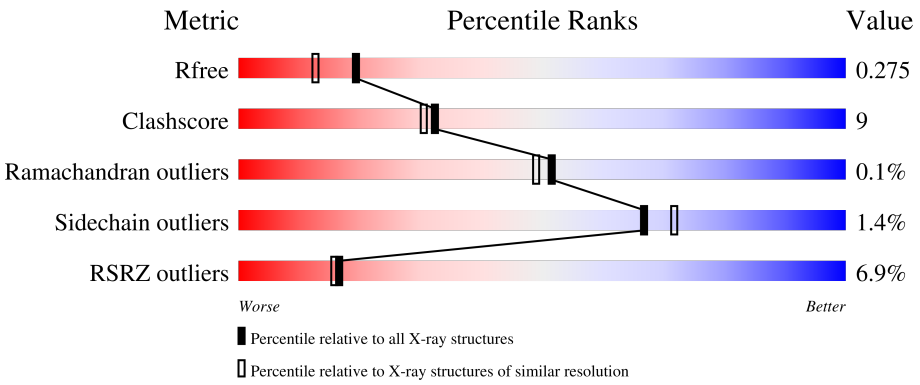
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	467	.% 76% 19% • •
1	B	467	2% 77% 19% •
1	C	467	13% 71% 22% 7%
1	D	467	10% 72% 19% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14692 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 Beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3559	2291	599	652	17	0	0	0
1	B	450	3582	2304	602	659	17	0	0	0
1	C	434	3462	2230	580	636	16	0	0	0
1	D	432	3429	2216	567	631	15	0	0	0

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
2	A	8	8	8	0	0
2	B	9	9	9	0	0
2	C	9	9	9	0	0
2	D	7	7	7	0	0

- Molecule 3 is water.

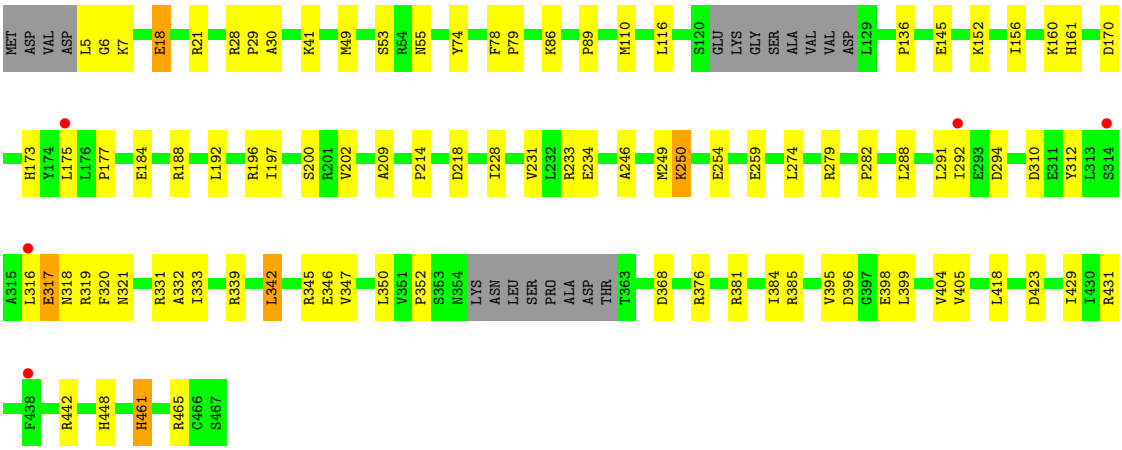
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	170	170	170	0	0
3	B	221	221	221	0	0
3	C	113	113	113	0	0
3	D	123	123	123	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

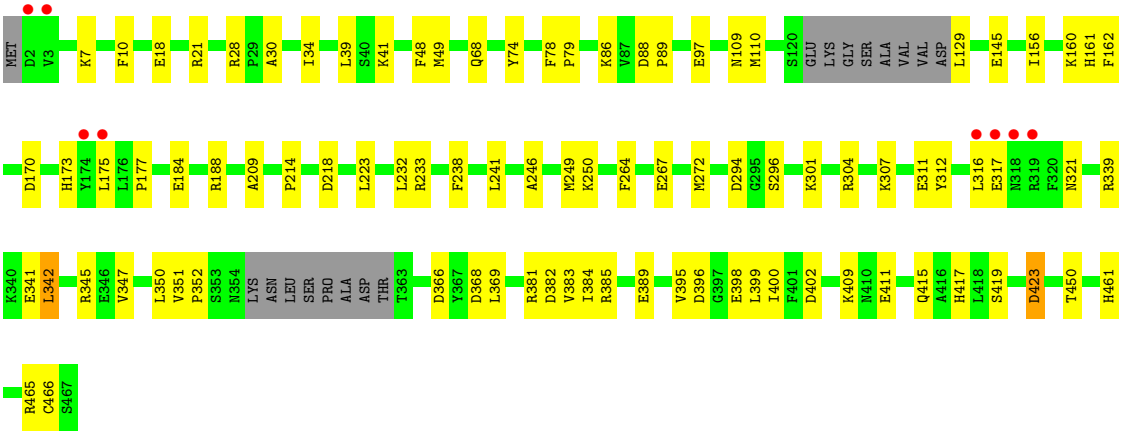
• Molecule 1: Beta-N-acetylhexosaminidase

Chain A:



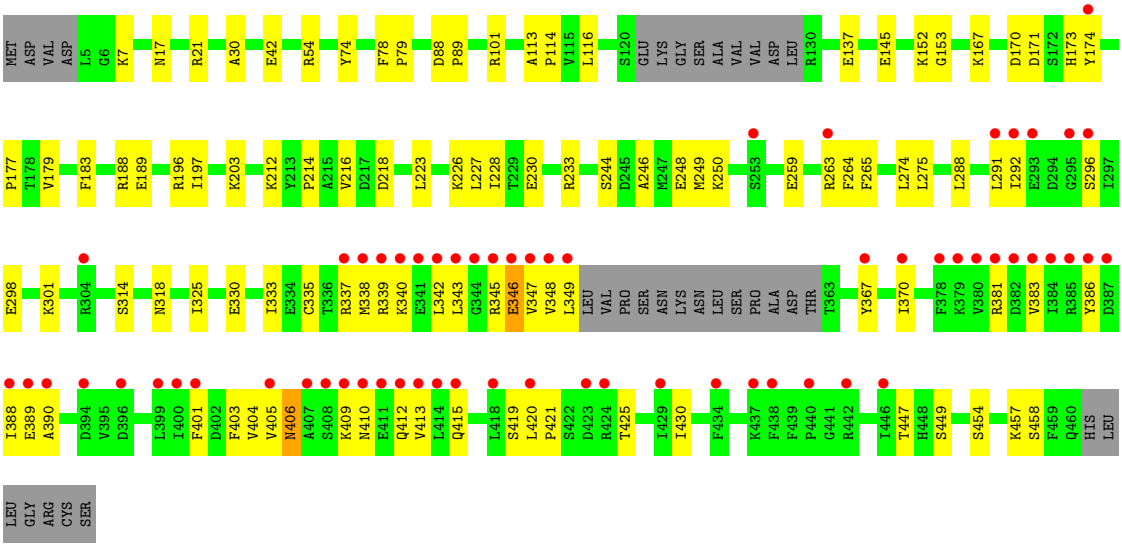
• Molecule 1: Beta-N-acetylhexosaminidase

Chain B:



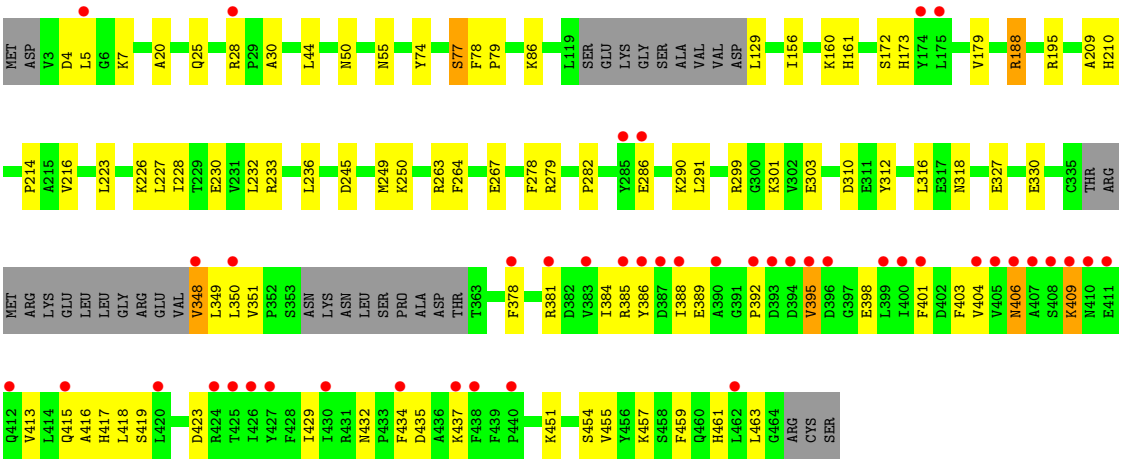
• Molecule 1: Beta-N-acetylhexosaminidase

Chain C:



- Molecule 1: Beta-N-acetylhexosaminidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	158.97Å 158.97Å 517.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.74 – 2.00 39.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.8 (39.74-2.00) 93.9 (39.74-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.238 , 0.276 0.239 , 0.275	Depositor DCC
R_{free} test set	2000 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14692	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7120e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CD

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	1/3636 (0.0%)	0.77	4/4906 (0.1%)
1	B	0.71	0/3659	0.76	2/4938 (0.0%)
1	C	0.58	0/3537	0.69	1/4771 (0.0%)
1	D	0.57	0/3505	0.67	2/4734 (0.0%)
All	All	0.65	1/14337 (0.0%)	0.73	9/19349 (0.0%)

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	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	GLU	CB-CG	5.09	1.61	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	LEU	CA-CB-CG	6.83	131.02	115.30
1	A	342	LEU	CA-CB-CG	6.07	129.25	115.30
1	D	188	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	D	5	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	342	LEU	CA-CB-CG	5.43	127.78	115.30
1	C	88	ASP	CB-CG-OD1	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	218	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	B	218	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	331	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	346	GLU	Peptide
1	D	409	LYS	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	3559	0	3556	62	1
1	B	3582	0	3573	61	1
1	C	3462	0	3454	64	1
1	D	3429	0	3411	65	1
2	A	8	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
2	D	7	0	0	0	0
3	A	170	0	0	5	0
3	B	221	0	0	12	0
3	C	113	0	0	4	0
3	D	123	0	0	3	0
All	All	14692	0	13994	247	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 9.

All (247) 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:C:337:ARG:NH1	1:C:338:MET:O	1.88	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:GLU:O	1:C:409:LYS:NZ	1.89	1.05
1:B:18:GLU:OE1	1:B:21:ARG:NH1	1.94	1.00
1:A:234:GLU:N	3:A:601:HOH:O	2.06	0.89
1:C:420:LEU:HD12	1:C:421:PRO:HD2	1.54	0.89
1:C:367:TYR:HA	1:C:370:ILE:HD12	1.55	0.87
1:D:86:LYS:NZ	3:D:601:HOH:O	2.07	0.87
1:A:368:ASP:OD1	1:A:385:ARG:NH2	2.08	0.86
1:B:368:ASP:OD1	1:B:385:ARG:NH2	2.10	0.84
1:D:389:GLU:OE1	1:D:409:LYS:NZ	2.11	0.84
1:B:233:ARG:NH1	3:B:603:HOH:O	2.12	0.83
1:D:50:ASN:HD21	1:D:327:GLU:HG2	1.41	0.83
1:B:28:ARG:NH1	3:B:601:HOH:O	2.10	0.82
1:C:415:GLN:O	1:C:419:SER:OG	1.97	0.82
1:A:7:LYS:NZ	1:A:310:ASP:OD1	2.11	0.81
1:A:339:ARG:NH2	1:A:423:ASP:O	2.12	0.81
1:A:28:ARG:HH12	1:A:55:ASN:HB3	1.50	0.76
1:A:461:HIS:CD2	1:A:465:ARG:HH11	2.04	0.75
1:B:466:CYS:SG	3:B:606:HOH:O	2.46	0.73
1:A:461:HIS:HD2	1:A:465:ARG:HH11	1.36	0.73
1:C:137:GLU:OE2	1:C:196:ARG:NH1	2.23	0.71
1:D:406:ASN:HD21	1:D:409:LYS:HB2	1.56	0.71
1:A:173:HIS:O	1:A:250:LYS:NZ	2.20	0.70
1:B:465:ARG:NH1	3:B:606:HOH:O	2.26	0.68
1:D:415:GLN:HA	1:D:418:LEU:HB2	1.75	0.68
1:B:184:GLU:OE2	1:B:188:ARG:NE	2.22	0.68
1:D:50:ASN:ND2	1:D:327:GLU:HG2	2.10	0.67
1:C:405:VAL:O	1:C:406:ASN:ND2	2.19	0.66
1:D:318:ASN:ND2	3:D:606:HOH:O	2.27	0.66
1:C:410:ASN:OD1	1:C:412:GLN:N	2.30	0.65
1:A:41:LYS:HE2	3:A:663:HOH:O	1.97	0.65
1:C:228:ILE:O	1:C:233:ARG:HG2	1.97	0.65
1:D:406:ASN:O	1:D:406:ASN:ND2	2.30	0.65
1:A:184:GLU:OE2	1:A:188:ARG:NH1	2.30	0.64
1:C:263:ARG:CZ	1:C:296:SER:HB3	2.28	0.64
1:B:381:ARG:NH2	1:B:398:GLU:OE2	2.32	0.63
1:B:241:LEU:HD11	1:B:272:MET:HG3	1.82	0.62
1:A:246:ALA:O	1:A:249:MET:HE3	1.99	0.61
1:B:339:ARG:NH2	1:B:423:ASP:O	2.32	0.61
1:B:465:ARG:NH2	3:B:602:HOH:O	2.12	0.61
1:D:388:ILE:HG13	1:D:389:GLU:HG2	1.83	0.60
1:C:386:TYR:OH	1:C:403:PHE:O	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:ILE:O	1:D:233:ARG:HG2	2.02	0.59
1:A:319:ARG:NH1	1:B:97:GLU:OE2	2.35	0.59
1:D:28:ARG:HH12	1:D:55:ASN:HB3	1.68	0.59
1:D:381:ARG:NH1	1:D:398:GLU:OE2	2.33	0.59
1:B:267:GLU:OE1	1:B:301:LYS:NZ	2.36	0.58
1:A:136:PRO:HB2	1:A:192:LEU:HD23	1.86	0.58
1:D:7:LYS:NZ	1:D:310:ASP:OD1	2.32	0.57
1:D:392:PRO:HD3	1:D:417:HIS:CE1	2.40	0.57
1:A:352:PRO:O	1:A:385:ARG:NH1	2.37	0.57
1:C:339:ARG:HE	1:C:342:LEU:HD11	1.69	0.56
1:B:89:PRO:HB2	1:B:145:GLU:HG3	1.86	0.56
1:D:349:LEU:HD22	1:D:403:PHE:HE2	1.71	0.56
1:C:263:ARG:HB2	1:C:291:LEU:HD13	1.87	0.55
1:B:307:LYS:NZ	1:B:311:GLU:OE1	2.33	0.55
1:B:321:ASN:HB3	3:B:625:HOH:O	2.05	0.55
1:C:226:LYS:O	1:C:230:GLU:HB2	2.06	0.55
1:C:246:ALA:O	1:C:249:MET:HE3	2.06	0.55
1:D:7:LYS:HA	1:D:30:ALA:HB2	1.87	0.55
1:A:74:TYR:HA	1:B:74:TYR:HA	1.87	0.55
1:B:246:ALA:O	1:B:249:MET:HE3	2.06	0.55
1:A:312:TYR:O	1:A:316:LEU:HG	2.07	0.55
1:A:461:HIS:CD2	1:A:465:ARG:HD3	2.42	0.55
1:B:294:ASP:OD1	1:B:296:SER:OG	2.21	0.55
1:C:54:ARG:NH2	3:C:604:HOH:O	2.38	0.54
1:A:170:ASP:HB3	1:A:175:LEU:HD11	1.89	0.54
1:A:116:LEU:HD11	1:A:197:ILE:HD12	1.88	0.54
1:C:223:LEU:HB3	1:C:264:PHE:HB3	1.89	0.54
1:A:318:ASN:ND2	1:A:320:PHE:O	2.41	0.54
1:D:216:VAL:O	1:D:226:LYS:HD3	2.08	0.54
1:A:461:HIS:NE2	1:A:465:ARG:HD3	2.23	0.53
1:A:259:GLU:HG3	1:A:291:LEU:HD21	1.89	0.53
1:C:167:LYS:NZ	1:C:189:GLU:OE1	2.34	0.53
1:A:161:HIS:HB2	1:A:209:ALA:HB2	1.90	0.53
1:C:349:LEU:HD12	1:C:383:VAL:HG22	1.90	0.53
1:D:25:GLN:HA	1:D:28:ARG:CZ	2.40	0.52
1:A:7:LYS:HA	1:A:30:ALA:HB2	1.91	0.52
1:D:404:VAL:HB	1:D:429:ILE:HD13	1.90	0.52
1:C:74:TYR:HA	1:D:74:TYR:HA	1.92	0.52
1:C:318:ASN:ND2	3:C:606:HOH:O	2.39	0.52
1:C:259:GLU:HG3	1:C:291:LEU:HD21	1.91	0.52
1:B:345:ARG:HD3	1:B:398:GLU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:PHE:CD1	1:B:79:PRO:HD2	2.45	0.51
1:D:415:GLN:O	1:D:419:SER:N	2.44	0.51
1:C:420:LEU:HD23	1:C:425:THR:HG21	1.93	0.51
1:A:228:ILE:O	1:A:233:ARG:HG2	2.10	0.51
1:D:349:LEU:HD23	1:D:401:PHE:HB2	1.92	0.51
1:B:170:ASP:HB2	1:B:177:PRO:HB3	1.91	0.51
1:A:404:VAL:HB	1:A:429:ILE:HD13	1.93	0.50
1:C:170:ASP:HB2	1:C:177:PRO:HB3	1.93	0.50
1:D:172:SER:HB2	1:D:249:MET:HE1	1.93	0.50
1:A:246:ALA:H	1:A:249:MET:HE2	1.76	0.50
1:B:304:ARG:HD3	3:B:682:HOH:O	2.10	0.50
1:C:298:GLU:OE1	1:C:301:LYS:NZ	2.40	0.50
1:D:299:ARG:O	1:D:303:GLU:HG3	2.11	0.50
1:C:330:GLU:HB2	1:C:457:LYS:HD2	1.94	0.49
1:A:294:ASP:OD1	1:A:294:ASP:C	2.51	0.49
1:C:248:GLU:OE2	1:C:275:LEU:HB3	2.11	0.49
1:C:389:GLU:C	1:C:409:LYS:HZ3	2.12	0.49
1:C:449:SER:HB3	1:C:454:SER:OG	2.12	0.49
1:D:378:PHE:CE1	1:D:463:LEU:HD21	2.47	0.49
1:A:345:ARG:HD3	1:A:398:GLU:HB3	1.93	0.49
1:A:418:LEU:O	1:A:442:ARG:NH2	2.45	0.49
1:D:78:PHE:CD1	1:D:79:PRO:HD2	2.48	0.49
1:D:286:GLU:O	1:D:290:LYS:HG2	2.12	0.49
1:A:250:LYS:HG2	1:A:254:GLU:HG3	1.95	0.49
1:C:337:ARG:HH12	1:C:340:LYS:H	1.60	0.49
1:D:432:ASN:HB3	1:D:435:ASP:OD2	2.13	0.49
1:D:312:TYR:O	1:D:316:LEU:HG	2.13	0.49
1:A:200:SER:OG	1:A:202:VAL:HG13	2.13	0.48
1:B:7:LYS:HA	1:B:30:ALA:HB2	1.96	0.48
1:C:430:ILE:HA	1:C:447:THR:OG1	2.14	0.48
1:A:53:SER:HB3	1:A:321:ASN:ND2	2.28	0.48
1:D:195:ARG:HG2	1:D:236:LEU:HD21	1.95	0.48
1:B:350:LEU:HD23	1:B:384:ILE:HB	1.94	0.48
1:C:389:GLU:C	1:C:409:LYS:NZ	2.64	0.48
1:D:161:HIS:HB2	1:D:209:ALA:HB2	1.96	0.48
1:C:345:ARG:C	1:C:346:GLU:HG3	2.34	0.48
1:B:382:ASP:OD1	1:B:383:VAL:N	2.47	0.48
1:A:18:GLU:OE1	1:A:21:ARG:NH2	2.40	0.48
1:D:20:ALA:HA	1:D:278:PHE:CE2	2.49	0.47
1:D:381:ARG:NH2	1:D:398:GLU:OE2	2.45	0.47
1:A:49:MET:HB3	1:A:321:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ARG:NH2	3:C:607:HOH:O	2.39	0.47
1:B:461:HIS:ND1	1:B:465:ARG:HD3	2.30	0.47
1:A:192:LEU:HD11	1:A:196:ARG:NH2	2.30	0.47
1:A:346:GLU:CD	1:A:381:ARG:HH21	2.18	0.47
1:C:216:VAL:O	1:C:226:LYS:HD3	2.14	0.46
1:D:173:HIS:O	1:D:250:LYS:HB2	2.14	0.46
3:B:792:HOH:O	1:C:203:LYS:HB2	2.16	0.46
1:A:28:ARG:HA	1:A:28:ARG:HD3	1.81	0.46
1:A:405:VAL:HG22	1:A:431:ARG:HG3	1.98	0.46
1:B:352:PRO:O	1:B:385:ARG:NH1	2.48	0.46
1:B:411:GLU:O	1:B:415:GLN:HG2	2.16	0.46
1:D:223:LEU:HB3	1:D:264:PHE:HB3	1.97	0.46
1:D:413:VAL:O	1:D:416:ALA:HB3	2.15	0.46
1:D:348:VAL:HG12	1:D:349:LEU:N	2.31	0.46
1:D:350:LEU:HD23	1:D:384:ILE:HB	1.97	0.46
1:D:350:LEU:HD13	1:D:392:PRO:HB3	1.98	0.46
1:A:78:PHE:CD1	1:A:79:PRO:HD2	2.51	0.46
1:A:339:ARG:HB2	1:A:342:LEU:HD13	1.98	0.46
1:A:288:LEU:O	1:A:292:ILE:HG13	2.16	0.46
1:A:350:LEU:HD23	1:A:384:ILE:HB	1.98	0.46
1:B:389:GLU:HB3	1:B:409:LYS:HZ2	1.80	0.45
1:D:226:LYS:O	1:D:230:GLU:HB2	2.17	0.45
1:D:263:ARG:HB2	1:D:291:LEU:HD13	1.98	0.45
1:D:179:VAL:O	1:D:214:PRO:HD2	2.16	0.45
1:D:279:ARG:O	1:D:282:PRO:HD2	2.17	0.45
1:D:386:TYR:OH	1:D:403:PHE:O	2.27	0.45
1:C:116:LEU:HD11	1:C:197:ILE:HD12	1.97	0.45
1:C:179:VAL:O	1:C:214:PRO:HD2	2.17	0.45
1:A:279:ARG:O	1:A:282:PRO:HD2	2.17	0.45
1:C:246:ALA:H	1:C:249:MET:HE2	1.82	0.44
1:A:28:ARG:NH1	1:A:55:ASN:O	2.51	0.44
1:A:246:ALA:HA	1:A:274:LEU:O	2.18	0.44
1:B:461:HIS:HB3	3:B:606:HOH:O	2.17	0.44
1:C:78:PHE:CD1	1:C:79:PRO:HD2	2.52	0.44
1:B:339:ARG:HB3	1:B:341:GLU:OE2	2.17	0.44
1:D:351:VAL:O	1:D:385:ARG:HA	2.18	0.44
1:B:402:ASP:OD2	1:B:417:HIS:ND1	2.35	0.44
1:D:210:HIS:NE2	1:D:245:ASP:HB3	2.33	0.44
1:B:41:LYS:HE2	3:B:726:HOH:O	2.18	0.44
1:A:259:GLU:CG	1:A:291:LEU:HD21	2.47	0.44
1:B:68:GLN:OE1	1:B:129:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ARG:CZ	3:B:603:HOH:O	2.60	0.44
1:B:238:PHE:HD2	3:B:603:HOH:O	2.01	0.44
1:C:173:HIS:O	1:C:250:LYS:HB2	2.17	0.44
1:A:333:ILE:N	3:A:603:HOH:O	2.50	0.43
1:A:395:VAL:HG22	1:A:396:ASP:H	1.82	0.43
1:C:347:VAL:HG11	1:C:401:PHE:CD2	2.53	0.43
1:C:349:LEU:HD22	1:C:403:PHE:HE2	1.83	0.43
1:B:395:VAL:HG22	1:B:396:ASP:H	1.83	0.43
1:B:461:HIS:CE1	1:B:465:ARG:HD3	2.53	0.43
1:A:152:LYS:NZ	3:A:623:HOH:O	2.52	0.43
1:A:196:ARG:HD2	3:D:612:HOH:O	2.18	0.43
1:C:212:LYS:HE3	1:C:218:ASP:O	2.19	0.43
1:D:4:ASP:OD1	1:D:4:ASP:N	2.51	0.43
1:A:231:VAL:C	3:A:601:HOH:O	2.57	0.43
1:A:246:ALA:N	1:A:249:MET:HE2	2.33	0.43
1:B:366:ASP:HB3	1:B:450:THR:O	2.19	0.43
1:B:415:GLN:O	1:B:419:SER:OG	2.30	0.43
1:D:228:ILE:O	1:D:232:LEU:HB3	2.18	0.43
1:D:434:PHE:HB3	1:D:437:LYS:NZ	2.34	0.43
1:D:129:LEU:HA	1:D:129:LEU:HD23	1.81	0.43
1:D:384:ILE:CD1	1:D:395:VAL:HG11	2.48	0.43
1:B:49:MET:HB3	1:B:321:ASN:OD1	2.19	0.42
1:C:171:ASP:HB3	1:C:174:TYR:HD2	1.83	0.42
1:C:113:ALA:HB1	1:C:114:PRO:HA	2.01	0.42
1:C:333:ILE:HD13	1:C:458:SER:HA	2.01	0.42
1:A:332:ALA:O	1:A:448:HIS:ND1	2.47	0.42
1:B:339:ARG:NH2	1:B:342:LEU:HD11	2.33	0.42
1:C:390:ALA:C	1:C:413:VAL:HG12	2.40	0.42
1:B:369:LEU:HD23	1:B:369:LEU:HA	1.92	0.42
1:A:6:GLY:O	1:A:29:PRO:HA	2.19	0.42
1:B:347:VAL:HG22	1:B:399:LEU:HD23	2.01	0.42
1:C:7:LYS:HA	1:C:30:ALA:HB2	2.01	0.42
1:C:405:VAL:C	1:C:406:ASN:HD22	2.14	0.42
1:B:156:ILE:HD12	1:B:316:LEU:HD21	2.01	0.42
1:B:161:HIS:HB2	1:B:209:ALA:HB2	2.02	0.42
1:B:173:HIS:O	1:B:250:LYS:HD2	2.19	0.42
1:B:223:LEU:HB3	1:B:264:PHE:HB3	2.01	0.42
1:C:246:ALA:HA	1:C:274:LEU:O	2.20	0.42
1:C:325:ILE:HG23	1:D:79:PRO:HD3	2.02	0.42
1:B:162:PHE:CZ	1:B:232:LEU:HB2	2.55	0.42
1:C:244:SER:HB3	1:C:265:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:PRO:HB2	1:C:145:GLU:HG3	2.01	0.41
1:D:156:ILE:CG1	1:D:316:LEU:HD21	2.48	0.41
1:B:160:LYS:HA	1:B:161:HIS:HA	1.83	0.41
1:D:299:ARG:NH2	1:D:303:GLU:OE2	2.53	0.41
1:D:455:VAL:HG12	1:D:459:PHE:CE2	2.55	0.41
1:D:7:LYS:HA	1:D:30:ALA:CB	2.50	0.41
1:D:267:GLU:OE1	1:D:301:LYS:NZ	2.50	0.41
1:B:109:ASN:CG	1:B:316:LEU:HD13	2.41	0.41
1:C:17:ASN:O	1:C:21:ARG:HG3	2.20	0.41
1:C:183:PHE:HB2	1:C:216:VAL:HG22	2.02	0.41
1:D:44:LEU:HD12	1:D:44:LEU:HA	1.89	0.41
1:D:437:LYS:HB2	1:D:437:LYS:HE2	1.87	0.41
1:C:339:ARG:HB2	1:C:342:LEU:HG	2.02	0.41
1:C:339:ARG:NE	1:C:342:LEU:HD11	2.35	0.41
1:B:175:LEU:O	1:B:177:PRO:HD3	2.20	0.41
1:D:160:LYS:HA	1:D:161:HIS:HA	1.89	0.41
1:A:86:LYS:HD2	1:A:86:LYS:HA	1.80	0.41
1:C:388:ILE:HG13	1:C:389:GLU:HG2	2.02	0.41
1:A:175:LEU:O	1:A:177:PRO:HD3	2.20	0.41
1:A:347:VAL:HG22	1:A:399:LEU:HD23	2.03	0.41
1:B:34:ILE:HG22	1:B:39:LEU:HG	2.02	0.41
1:B:88:ASP:HA	1:B:89:PRO:HD2	1.94	0.41
1:B:368:ASP:HA	1:B:385:ARG:NH2	2.35	0.41
1:B:396:ASP:HA	1:B:400:ILE:HD11	2.02	0.41
1:D:227:LEU:HD23	1:D:227:LEU:HA	1.90	0.41
1:A:89:PRO:HB2	1:A:145:GLU:HG3	2.02	0.41
1:B:110:MET:HG3	1:B:156:ILE:O	2.20	0.41
1:C:42:GLU:OE1	1:D:77:SER:HB2	2.20	0.41
1:C:288:LEU:O	1:C:292:ILE:HG13	2.21	0.41
1:A:160:LYS:HA	1:A:161:HIS:HA	1.88	0.40
1:D:457:LYS:HD3	1:D:457:LYS:HA	1.94	0.40
1:A:110:MET:HG3	1:A:156:ILE:O	2.20	0.40
1:B:351:VAL:O	1:B:385:ARG:HA	2.21	0.40
1:C:152:LYS:HE2	3:C:690:HOH:O	2.21	0.40
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.91	0.40
1:B:312:TYR:O	1:B:316:LEU:HG	2.20	0.40
1:C:101:ARG:HA	1:C:153:GLY:O	2.21	0.40
1:A:196:ARG:HA	1:A:196:ARG:HD3	1.92	0.40
1:B:294:ASP:OD1	1:B:294:ASP:C	2.60	0.40
1:D:330:GLU:HB2	1:D:457:LYS:HD2	2.04	0.40
1:D:451:LYS:O	1:D:454:SER:HB2	2.22	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)
1:A:214:PRO:O	1:D:188:ARG:NH1[4_556]	1.94	0.26
1:B:214:PRO:O	1:C:188:ARG:NH1[18_655]	2.04	0.16

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	441/467 (94%)	427 (97%)	13 (3%)	1 (0%)	47	44
1	B	444/467 (95%)	430 (97%)	13 (3%)	1 (0%)	47	44
1	C	428/467 (92%)	417 (97%)	11 (3%)	0	100	100
1	D	424/467 (91%)	413 (97%)	11 (3%)	0	100	100
All	All	1737/1868 (93%)	1687 (97%)	48 (3%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	317	GLU
1	A	317	GLU

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	389/406 (96%)	385 (99%)	4 (1%)	76	81
1	B	392/406 (97%)	388 (99%)	4 (1%)	76	81
1	C	377/406 (93%)	370 (98%)	7 (2%)	57	61
1	D	374/406 (92%)	368 (98%)	6 (2%)	62	67
All	All	1532/1624 (94%)	1511 (99%)	21 (1%)	67	72

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	LYS
1	A	317	GLU
1	A	376	ARG
1	A	461	HIS
1	B	10	PHE
1	B	48	PHE
1	B	86	LYS
1	B	423	ASP
1	C	314	SER
1	C	335	CYS
1	C	343	LEU
1	C	348	VAL
1	C	381	ARG
1	C	404	VAL
1	C	406	ASN
1	D	77	SER
1	D	348	VAL
1	D	395	VAL
1	D	406	ASN
1	D	423	ASP
1	D	461	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	50	ASN
1	D	406	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 33 are monoatomic - leaving 0 for Mogul analysis.

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.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	447/467 (95%)	-0.05	5 (1%)	80	79	8, 17, 37, 68	0
1	B	450/467 (96%)	-0.04	8 (1%)	68	66	7, 17, 41, 67	0
1	C	434/467 (92%)	0.71	63 (14%)	2	2	10, 32, 117, 152	0
1	D	432/467 (92%)	0.47	45 (10%)	6	5	10, 28, 94, 115	0
All	All	1763/1868 (94%)	0.27	121 (6%)	16	16	7, 22, 89, 152	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	343	LEU	9.3
1	C	378	PHE	7.1
1	C	383	VAL	6.3
1	C	399	LEU	5.9
1	D	388	ILE	5.8
1	C	346	GLU	5.8
1	C	342	LEU	5.7
1	C	341	GLU	5.7
1	D	424	ARG	5.4
1	C	400	ILE	5.4
1	C	344	GLY	5.1
1	C	338	MET	5.1
1	D	395	VAL	5.1
1	C	380	VAL	5.0
1	C	381	ARG	4.9
1	D	407	ALA	4.8
1	C	349	LEU	4.8
1	D	350	LEU	4.7
1	C	379	LYS	4.6
1	C	424	ARG	4.5
1	D	381	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	400	ILE	4.4
1	D	383	VAL	4.3
1	D	378	PHE	4.3
1	D	409	LYS	4.2
1	C	345	ARG	4.2
1	C	339	ARG	4.1
1	C	386	TYR	4.0
1	C	347	VAL	4.0
1	D	392	PRO	4.0
1	C	388	ILE	4.0
1	C	408	SER	3.9
1	C	412	GLN	3.9
1	C	420	LEU	3.9
1	C	394	ASP	3.9
1	C	409	LYS	3.8
1	C	437	LYS	3.8
1	C	390	ALA	3.7
1	C	407	ALA	3.7
1	C	340	LYS	3.6
1	C	401	PHE	3.6
1	D	386	TYR	3.6
1	D	425	THR	3.6
1	C	174	TYR	3.5
1	C	337	ARG	3.5
1	D	175	LEU	3.4
1	C	367	TYR	3.4
1	D	390	ALA	3.4
1	B	174	TYR	3.3
1	C	423	ASP	3.3
1	D	427	TYR	3.2
1	D	348	VAL	3.1
1	C	384	ILE	3.1
1	C	413	VAL	3.0
1	C	429	ILE	2.9
1	C	293	GLU	2.9
1	C	434	PHE	2.9
1	C	405	VAL	2.8
1	D	406	ASN	2.8
1	C	438	PHE	2.8
1	D	438	PHE	2.8
1	D	401	PHE	2.8
1	A	314	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	410	ASN	2.8
1	B	2	ASP	2.7
1	C	440	PRO	2.6
1	C	304	ARG	2.6
1	C	385	ARG	2.6
1	D	410	ASN	2.6
1	A	316	LEU	2.6
1	D	393	ASP	2.5
1	D	420	LEU	2.6
1	C	296	SER	2.5
1	D	411	GLU	2.5
1	B	175	LEU	2.5
1	C	415	GLN	2.5
1	D	434	PHE	2.5
1	C	263	ARG	2.5
1	C	292	ILE	2.5
1	A	438	PHE	2.4
1	C	382	ASP	2.4
1	D	408	SER	2.4
1	D	430	ILE	2.4
1	B	317	GLU	2.3
1	D	404	VAL	2.3
1	C	396	ASP	2.3
1	D	412	GLN	2.3
1	D	440	PRO	2.3
1	D	174	TYR	2.3
1	C	414	LEU	2.3
1	D	399	LEU	2.3
1	D	385	ARG	2.3
1	C	387	ASP	2.3
1	D	462	LEU	2.3
1	C	348	VAL	2.2
1	C	253	SER	2.2
1	D	415	GLN	2.2
1	D	437	LYS	2.2
1	D	286	GLU	2.2
1	B	3	VAL	2.2
1	C	411	GLU	2.2
1	B	318	ASN	2.2
1	B	316	LEU	2.2
1	D	405	VAL	2.2
1	D	396	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	387	ASP	2.1
1	A	292	ILE	2.1
1	C	370	ILE	2.1
1	C	295	GLY	2.1
1	C	291	LEU	2.1
1	D	5	LEU	2.1
1	D	285	TYR	2.1
1	B	319	ARG	2.0
1	C	446	ILE	2.0
1	D	426	ILE	2.0
1	A	175	LEU	2.0
1	C	418	LEU	2.0
1	C	389	GLU	2.0
1	C	442	ARG	2.0
1	D	28	ARG	2.0
1	D	394	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CD	C	501	1/1	0.49	0.10	134,134,134,134	0
2	CD	C	509	1/1	0.82	0.05	124,124,124,124	0
2	CD	C	507	1/1	0.84	0.11	85,85,85,85	0
2	CD	D	501	1/1	0.86	0.04	83,83,83,83	0
2	CD	B	506	1/1	0.87	0.05	105,105,105,105	0
2	CD	D	507	1/1	0.88	0.04	116,116,116,116	0
2	CD	B	509	1/1	0.90	0.04	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CD	C	506	1/1	0.91	0.03	119,119,119,119	0
2	CD	C	508	1/1	0.92	0.07	88,88,88,88	0
2	CD	C	504	1/1	0.92	0.05	105,105,105,105	0
2	CD	B	505	1/1	0.92	0.04	119,119,119,119	0
2	CD	A	503	1/1	0.92	0.09	115,115,115,115	0
2	CD	B	504	1/1	0.93	0.07	105,105,105,105	0
2	CD	A	507	1/1	0.94	0.05	78,78,78,78	0
2	CD	D	503	1/1	0.95	0.06	65,65,65,65	0
2	CD	A	508	1/1	0.95	0.06	95,95,95,95	0
2	CD	A	501	1/1	0.96	0.14	64,64,64,64	0
2	CD	D	505	1/1	0.96	0.03	99,99,99,99	0
2	CD	B	507	1/1	0.96	0.09	71,71,71,71	0
2	CD	C	503	1/1	0.97	0.08	74,74,74,74	0
2	CD	A	502	1/1	0.97	0.07	69,69,69,69	0
2	CD	A	504	1/1	0.97	0.03	98,98,98,98	0
2	CD	B	501	1/1	0.97	0.04	74,74,74,74	0
2	CD	C	502	1/1	0.97	0.10	52,52,52,52	0
2	CD	D	506	1/1	0.98	0.10	74,74,74,74	0
2	CD	B	502	1/1	0.98	0.13	48,48,48,48	0
2	CD	C	505	1/1	0.99	0.12	20,20,20,20	0
2	CD	D	502	1/1	0.99	0.11	46,46,46,46	0
2	CD	B	503	1/1	0.99	0.07	56,56,56,56	0
2	CD	A	505	1/1	0.99	0.09	60,60,60,60	0
2	CD	B	508	1/1	0.99	0.09	26,26,26,26	0
2	CD	A	506	1/1	0.99	0.11	21,21,21,21	0
2	CD	D	504	1/1	1.00	0.10	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.