



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:16 PM UTC

PDB ID : 5BZA / pdb_00005bza
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

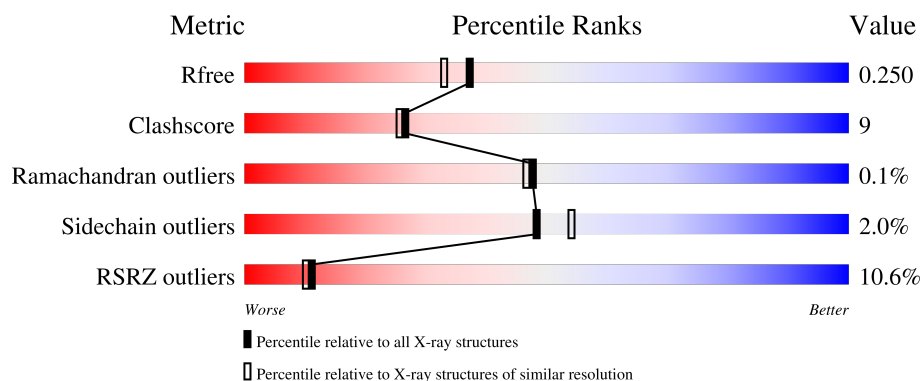
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	467	75% 19% • •
1	B	467	76% 20% •
1	C	467	22% 69% 23% • 7%
1	D	467	15% 71% 19% • 7%

2 Entry composition

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

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

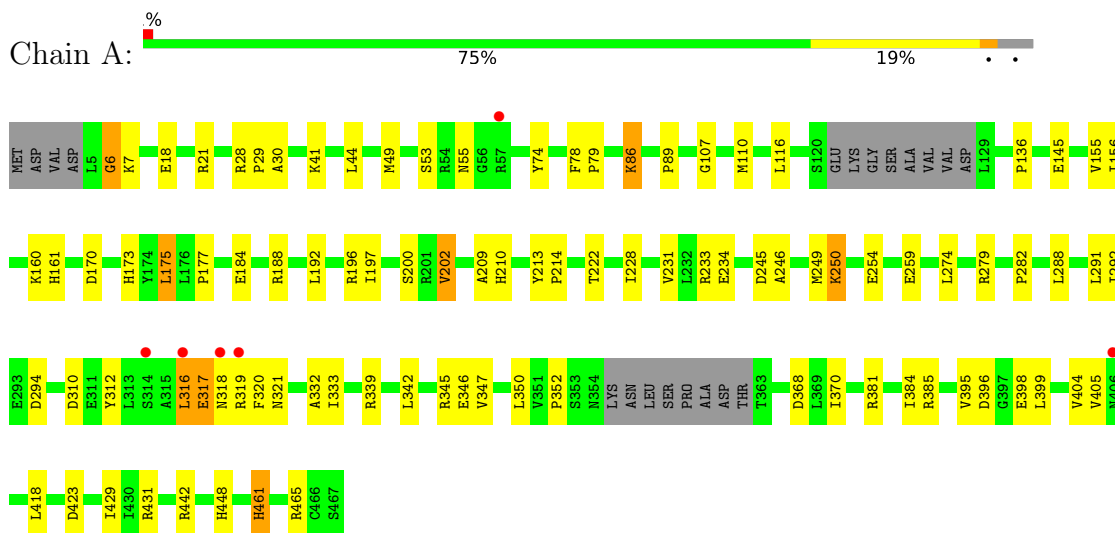
- Molecule 3 is water.

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

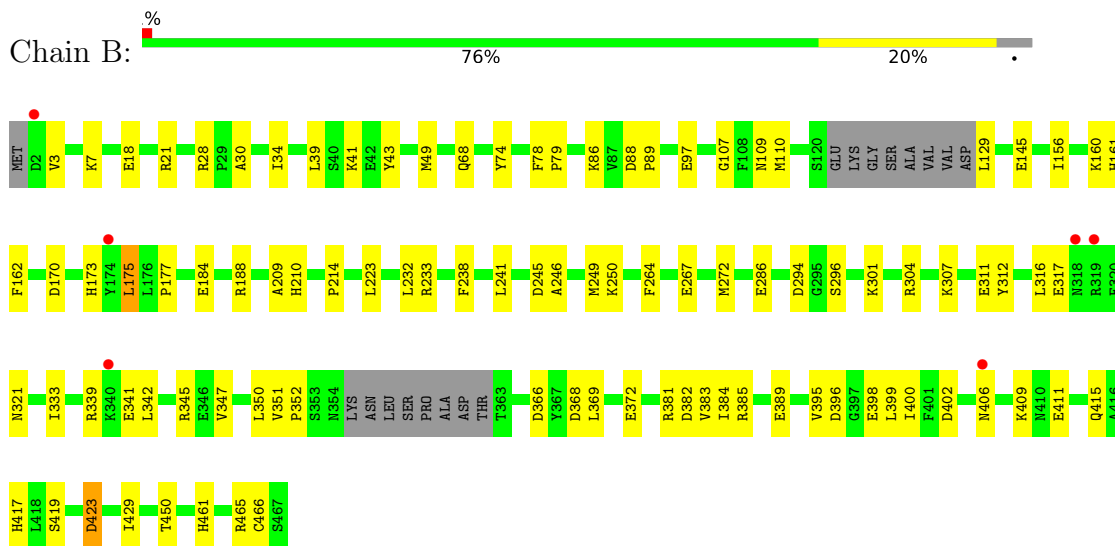
3 Residue-property plots

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

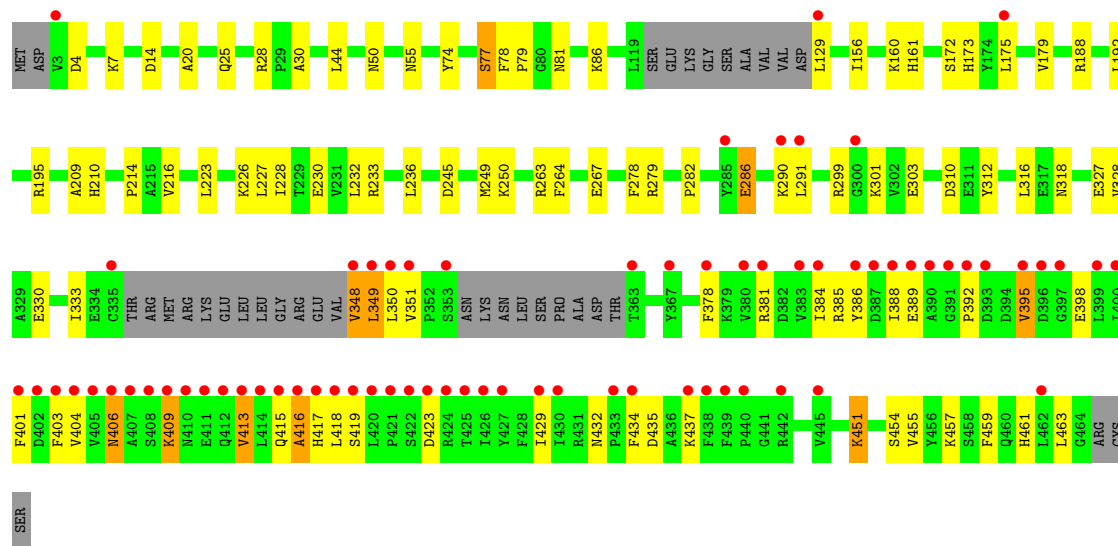


• Molecule 1: Beta-N-acetylhexosaminidase



• Molecule 1: Beta-N-acetylhexosaminidase





4 Data and refinement statistics

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) 93.8 (39.74-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.238 , 0.276 (Not available) , 0.250	Depositor DCC
R_{free} test set	2000 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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: 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	0.85	1/3636 (0.0%)	1.03	4/4906 (0.1%)
1	B	0.85	0/3659	1.03	2/4938 (0.0%)
1	C	0.69	0/3537	1.00	3/4771 (0.1%)
1	D	0.68	0/3505	0.98	10/4734 (0.2%)
All	All	0.78	1/14337 (0.0%)	1.01	19/19349 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	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	370	ILE	CA-CB	6.19	1.57	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	VAL	N-CA-C	6.34	117.72	108.53
1	A	316	LEU	N-CA-C	6.11	120.87	113.17
1	A	213	TYR	CA-C-N	6.01	126.17	119.32
1	A	213	TYR	C-N-CA	6.01	126.17	119.32
1	D	349	LEU	N-CA-C	5.82	118.59	108.76
1	C	336	THR	N-CA-C	-5.71	103.39	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	416	ALA	N-CA-C	-5.71	105.06	111.28
1	D	286	GLU	N-CA-C	-5.58	105.28	111.36
1	D	81	ASN	N-CA-C	5.37	117.13	111.28
1	B	3	VAL	N-CA-C	-5.32	106.33	112.98
1	C	412	GLN	N-CA-C	5.32	118.93	112.23
1	D	328	VAL	N-CA-C	-5.29	105.22	110.62
1	A	6	GLY	N-CA-C	-5.27	107.25	113.99
1	D	451	LYS	CA-C-N	5.22	125.27	119.32
1	D	451	LYS	C-N-CA	5.22	125.27	119.32
1	D	192	LEU	CA-C-N	-5.18	113.21	118.85
1	D	192	LEU	C-N-CA	-5.18	113.21	118.85
1	B	286	GLU	N-CA-C	-5.12	105.78	111.36
1	D	14	ASP	N-CA-C	-5.09	106.76	113.17

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	63	1
1	B	3582	0	3573	67	1
1	C	3462	0	3454	68	1
1	D	3429	0	3411	68	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	4	0
3	B	221	0	0	12	0
3	C	113	0	0	4	0
3	D	123	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14692	0	13994	261	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 (261) 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
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: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:A:49:MET:HE2	1:A:107:GLY:HA3	1.73	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:B:245:ASP:CG	1:B:249:MET:HE1	2.20	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:245:ASP:CG	1:C:249:MET:HE1	2.24	0.62
1:B:241:LEU:HD11	1:B:272:MET:HG3	1.82	0.62
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:A:245:ASP:CG	1:A:249:MET:HE1	2.26	0.60
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
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:A:210:HIS:CD2	1:A:249:MET:HE3	2.37	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:D:173:HIS:CE1	1:D:249:MET:HE3	2.39	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:246:ALA:HB3	1:B:249:MET:HE2	1.87	0.56
1:B:49:MET:HE2	1:B:107:GLY:HA3	1.88	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: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:A:312:TYR:O	1:A:316:LEU:HG	2.07	0.55
1:C:49:MET:HE2	1:C:107:GLY:HA3	1.86	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:C:389:GLU:C	1:C:409:LYS:HZ3	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:LEU:HB3	1:C:264:PHE:HB3	1.89	0.54
1:A:294:ASP:OD1	1:A:294:ASP:C	2.51	0.54
1:C:246:ALA:HB3	1:C:249:MET:HE2	1.90	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:43:TYR:OH	1:C:372:GLU:OE2	2.19	0.53
1:C:349:LEU:HD12	1:C:383:VAL:HG22	1.90	0.53
1:C:389:GLU:C	1:C:409:LYS:NZ	2.64	0.53
1:C:298:GLU:OE1	1:C:301:LYS:NZ	2.40	0.53
1:C:345:ARG:C	1:C:346:GLU:HG3	2.34	0.53
1:D:25:GLN:HA	1:D:28:ARG:CZ	2.40	0.52
1:A:246:ALA:HB3	1:A:249:MET:HE2	1.91	0.52
1:A:7:LYS:HA	1:A:30:ALA:HB2	1.91	0.52
1:C:405:VAL:C	1:C:406:ASN:HD22	2.14	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
1:B:78:PHE:CD1	1:B:79:PRO:HD2	2.45	0.51
1:A:346:GLU:CD	1:A:381:ARG:HH21	2.18	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:D:86:LYS:NZ	3:D:601:HOH:O	2.07	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:B:304:ARG:HD3	3:B:682:HOH:O	2.10	0.50
1:C:210:HIS:CD2	1:C:249:MET:HE3	2.47	0.50
1:D:299:ARG:O	1:D:303:GLU:HG3	2.11	0.50
1:B:210:HIS:CD2	1:B:249:MET:HE3	2.47	0.50
1:B:461:HIS:HD1	1:B:465:ARG:HD3	1.77	0.50
1:C:330:GLU:HB2	1:C:457:LYS:HD2	1.94	0.49
1:C:248:GLU:OE2	1:C:275:LEU:HB3	2.11	0.49
1:C:449:SER:HB3	1:C:454:SER:OG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:161:HIS:HB2	1:D:209:ALA:HB2	1.96	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:A:231:VAL:C	3:A:601:HOH:O	2.57	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
1:C:390:ALA:C	1:C:413:VAL:HG12	2.40	0.47
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:D:173:HIS:ND1	1:D:249:MET:HE3	2.30	0.47
1:A:192:LEU:HD11	1:A:196:ARG:NH2	2.30	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:B:109:ASN:CG	1:B:316:LEU:HD13	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.46
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:D:381:ARG:HH12	1:D:398:GLU:CD	2.24	0.45
1:B:294:ASP:OD1	1:B:294:ASP:C	2.60	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
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: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:B:366:ASP:HB3	1:B:450:THR:O	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:43:TYR:OH	1:B:372:GLU:OE2	2.32	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:B:406:ASN:CG	1:B:406:ASN:O	2.62	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: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
1:B:415:GLN:O	1:B:419:SER:OG	2.30	0.41
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: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:C:294:ASP:OD1	1:C:294:ASP:C	2.63	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:A:210:HIS:ND1	1:A:222:THR:OG1	2.50	0.41
1:C:388:ILE:HG13	1:C:389:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:SER:HB2	1:D:249:MET:HE2	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: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%)	43	42
1	B	444/467 (95%)	430 (97%)	13 (3%)	1 (0%)	43	42
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%)	48	46

All (2) Ramachandran outliers are listed below:

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

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	372/406 (92%)	364 (98%)	8 (2%)	45	50
1	B	392/406 (97%)	387 (99%)	5 (1%)	61	68
1	C	377/406 (93%)	368 (98%)	9 (2%)	43	47
1	D	374/406 (92%)	365 (98%)	9 (2%)	43	47
All	All	1515/1624 (93%)	1484 (98%)	31 (2%)	48	54

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	86	LYS
1	A	155	VAL
1	A	175	LEU
1	A	202	VAL
1	A	250	LYS
1	A	317	GLU

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Mol	Chain	Res	Type
1	A	461	HIS
1	B	86	LYS
1	B	175	LEU
1	B	333	ILE
1	B	423	ASP
1	B	429	ILE
1	C	175	LEU
1	C	314	SER
1	C	333	ILE
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	175	LEU
1	D	333	ILE
1	D	348	VAL
1	D	395	VAL
1	D	406	ASN
1	D	413	VAL
1	D	423	ASP
1	D	461	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	104	ASN
1	B	173	HIS
1	B	432	ASN
1	C	25	GLN
1	C	50	ASN
1	C	173	HIS
1	C	180	ASN
1	D	50	ASN
1	D	68	GLN
1	D	104	ASN
1	D	180	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 oligosaccharides 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

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	447/467 (95%)	-0.22	6 (1%) 75 74	8, 17, 37, 68	0
1	B	450/467 (96%)	-0.19	6 (1%) 75 74	7, 17, 41, 67	0
1	C	434/467 (92%)	0.95	103 (23%) 2 2	10, 32, 117, 152	0
1	D	432/467 (92%)	0.61	71 (16%) 4 4	10, 28, 94, 115	0
All	All	1763/1868 (94%)	0.28	186 (10%) 11 10	7, 22, 89, 152	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	399	LEU	9.5
1	C	395	VAL	7.3
1	C	378	PHE	7.2
1	C	343	LEU	6.7
1	D	390	ALA	6.4
1	D	395	VAL	6.3
1	C	342	LEU	6.3
1	C	407	ALA	6.3
1	D	418	LEU	6.1
1	C	388	ILE	6.0
1	D	388	ILE	6.0
1	D	348	VAL	5.9
1	C	418	LEU	5.9
1	C	349	LEU	5.7
1	D	407	ALA	5.7
1	C	401	PHE	5.6
1	D	350	LEU	5.6
1	C	386	TYR	5.6
1	C	426	ILE	5.3
1	C	390	ALA	5.3
1	C	400	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	340	LYS	5.0
1	C	347	VAL	5.0
1	D	384	ILE	5.0
1	D	399	LEU	4.9
1	C	384	ILE	4.8
1	C	438	PHE	4.7
1	C	397	GLY	4.5
1	C	422	SER	4.5
1	C	414	LEU	4.5
1	C	429	ILE	4.4
1	C	344	GLY	4.4
1	C	383	VAL	4.4
1	C	408	SER	4.3
1	C	380	VAL	4.2
1	D	414	LEU	4.2
1	C	346	GLU	4.2
1	D	397	GLY	4.1
1	C	394	ASP	4.1
1	C	348	VAL	4.1
1	C	385	ARG	4.0
1	D	400	ILE	4.0
1	C	363	THR	4.0
1	D	386	TYR	3.9
1	C	345	ARG	3.9
1	C	413	VAL	3.9
1	D	392	PRO	3.9
1	D	378	PHE	3.9
1	D	413	VAL	3.8
1	C	420	LEU	3.8
1	D	405	VAL	3.8
1	D	420	LEU	3.8
1	C	398	GLU	3.8
1	C	409	LYS	3.8
1	C	439	PHE	3.8
1	D	3	VAL	3.7
1	D	383	VAL	3.7
1	C	410	ASN	3.7
1	D	401	PHE	3.7
1	C	444	VAL	3.6
1	D	426	ILE	3.6
1	C	419	SER	3.6
1	C	396	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	427	TYR	3.5
1	C	428	PHE	3.5
1	D	427	TYR	3.5
1	C	405	VAL	3.5
1	D	425	THR	3.4
1	C	389	GLU	3.4
1	C	440	PRO	3.4
1	D	396	ASP	3.4
1	C	337	ARG	3.4
1	C	381	ARG	3.4
1	C	421	PRO	3.4
1	C	402	ASP	3.3
1	C	445	VAL	3.3
1	C	423	ASP	3.3
1	C	417	HIS	3.3
1	C	339	ARG	3.3
1	C	379	LYS	3.3
1	C	392	PRO	3.3
1	C	441	GLY	3.3
1	D	404	VAL	3.3
1	D	438	PHE	3.3
1	D	393	ASP	3.3
1	C	415	GLN	3.2
1	D	421	PRO	3.2
1	D	353	SER	3.2
1	C	391	GLY	3.2
1	C	404	VAL	3.2
1	D	391	GLY	3.2
1	C	258	VAL	3.1
1	D	381	ARG	3.1
1	C	341	GLU	3.1
1	C	433	PRO	3.0
1	C	336	THR	3.0
1	C	403	PHE	3.0
1	D	417	HIS	3.0
1	D	439	PHE	3.0
1	C	424	ARG	3.0
1	D	416	ALA	3.0
1	C	412	GLN	2.9
1	D	434	PHE	3.0
1	D	422	SER	2.9
1	D	349	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	295	GLY	2.9
1	C	174	TYR	2.9
1	C	434	PHE	2.9
1	D	424	ARG	2.9
1	A	314	SER	2.9
1	A	406	ASN	2.9
1	A	316	LEU	2.8
1	C	436	ALA	2.8
1	C	367	TYR	2.8
1	D	389	GLU	2.8
1	D	433	PRO	2.8
1	C	370	ILE	2.8
1	D	363	THR	2.8
1	C	437	LYS	2.7
1	C	406	ASN	2.7
1	C	393	ASP	2.7
1	C	446	ILE	2.7
1	C	442	ARG	2.7
1	D	462	LEU	2.7
1	B	174	TYR	2.7
1	B	318	ASN	2.7
1	C	425	THR	2.6
1	A	318	ASN	2.6
1	D	410	ASN	2.6
1	D	335	CYS	2.6
1	C	443	SER	2.6
1	D	415	GLN	2.6
1	D	445	VAL	2.6
1	D	300	GLY	2.6
1	C	253	SER	2.6
1	C	377	PHE	2.5
1	C	292	ILE	2.5
1	D	367	TYR	2.5
1	C	294	ASP	2.5
1	B	319	ARG	2.5
1	D	409	LYS	2.5
1	C	296	SER	2.4
1	C	338	MET	2.4
1	D	412	GLN	2.4
1	D	175	LEU	2.4
1	C	430	ILE	2.4
1	D	437	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	293	GLU	2.4
1	D	408	SER	2.4
1	B	406	ASN	2.3
1	D	423	ASP	2.3
1	D	419	SER	2.3
1	C	319	ARG	2.3
1	C	411	GLU	2.3
1	D	380	VAL	2.3
1	C	263	ARG	2.3
1	D	387	ASP	2.3
1	D	402	ASP	2.3
1	D	442	ARG	2.3
1	D	429	ILE	2.3
1	D	403	PHE	2.2
1	D	406	ASN	2.2
1	D	290	LYS	2.2
1	C	335	CYS	2.2
1	C	416	ALA	2.2
1	D	430	ILE	2.2
1	C	387	ASP	2.2
1	C	284	TYR	2.2
1	A	57	ARG	2.2
1	C	299	ARG	2.2
1	C	432	ASN	2.1
1	D	285	TYR	2.1
1	C	435	ASP	2.1
1	A	319	ARG	2.1
1	C	251	ALA	2.1
1	D	129	LEU	2.1
1	C	285	TYR	2.1
1	C	51	PHE	2.1
1	C	9	PHE	2.1
1	C	264	PHE	2.1
1	D	351	VAL	2.1
1	D	411	GLU	2.0
1	B	2	ASP	2.0
1	D	440	PRO	2.0
1	D	291	LEU	2.0
1	B	340	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	C	509	1/1	0.78	0.10	124,124,124,124	0
2	CD	B	506	1/1	0.87	0.11	105,105,105,105	0
2	CD	B	509	1/1	0.90	0.08	98,98,98,98	0
2	CD	B	505	1/1	0.91	0.09	119,119,119,119	0
2	CD	B	504	1/1	0.91	0.09	105,105,105,105	0
2	CD	C	501	1/1	0.92	0.13	134,134,134,134	0
2	CD	D	501	1/1	0.92	0.10	83,83,83,83	0
2	CD	C	504	1/1	0.93	0.10	105,105,105,105	0
2	CD	C	506	1/1	0.93	0.06	119,119,119,119	0
2	CD	D	507	1/1	0.93	0.06	116,116,116,116	0
2	CD	A	504	1/1	0.94	0.08	98,98,98,98	0
2	CD	A	502	1/1	0.94	0.07	69,69,69,69	0
2	CD	C	507	1/1	0.94	0.06	85,85,85,85	0
2	CD	C	508	1/1	0.95	0.08	88,88,88,88	0
2	CD	A	503	1/1	0.95	0.07	115,115,115,115	0
2	CD	A	507	1/1	0.96	0.08	78,78,78,78	0
2	CD	A	508	1/1	0.96	0.08	95,95,95,95	0
2	CD	D	505	1/1	0.96	0.05	99,99,99,99	0
2	CD	B	501	1/1	0.96	0.07	74,74,74,74	0
2	CD	C	503	1/1	0.97	0.04	74,74,74,74	0
2	CD	B	502	1/1	0.97	0.04	48,48,48,48	0
2	CD	A	501	1/1	0.97	0.05	64,64,64,64	0
2	CD	D	502	1/1	0.98	0.03	46,46,46,46	0
2	CD	D	503	1/1	0.98	0.04	65,65,65,65	0
2	CD	C	502	1/1	0.98	0.03	52,52,52,52	0
2	CD	A	505	1/1	0.98	0.03	60,60,60,60	0
2	CD	B	507	1/1	0.99	0.03	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	B	503	1/1	0.99	0.03	56,56,56,56	0
2	CD	D	506	1/1	0.99	0.03	74,74,74,74	0
2	CD	C	505	1/1	0.99	0.04	20,20,20,20	0
2	CD	B	508	1/1	1.00	0.01	26,26,26,26	0
2	CD	A	506	1/1	1.00	0.03	21,21,21,21	0
2	CD	D	504	1/1	1.00	0.02	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.