



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:45 PM UTC

PDB ID : 2RAG / pdb_00002rag
Title : Crystal structure of aminohydrolase from *Caulobacter crescentus*
Authors : Fedorov, A.A.; Fedorov, E.V.; Toro, R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-09-14
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
Xtrriage (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

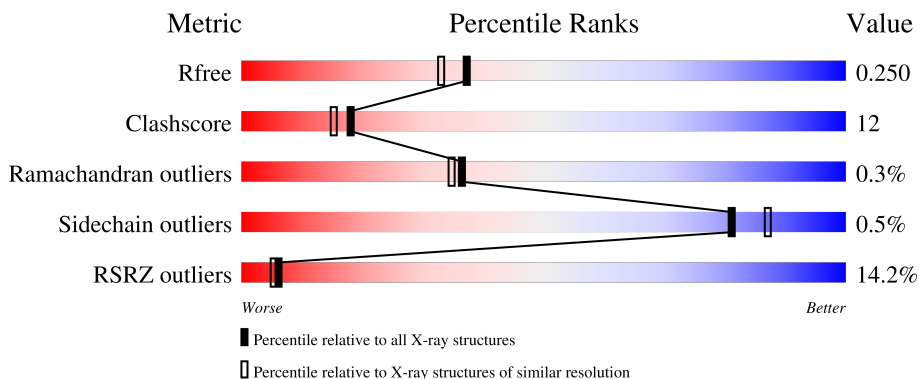
1 Overall quality at a glance

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	417	
1	B	417	
1	C	417	
1	D	417	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11860 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 Dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	369	2831	1783	492	545	11	0	0	0
1	B	369	2831	1783	492	545	11	0	0	0
1	C	369	2831	1783	492	545	11	0	0	0
1	D	369	2831	1783	492	545	11	0	0	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

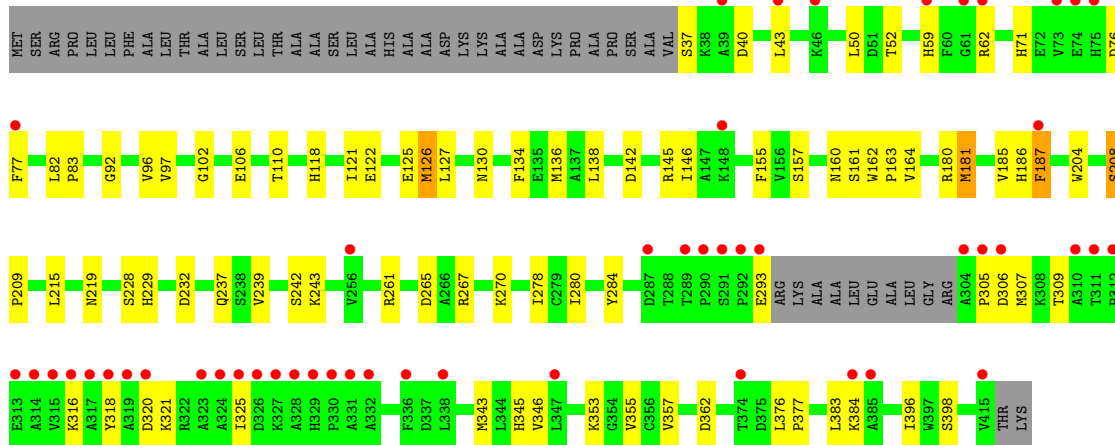
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

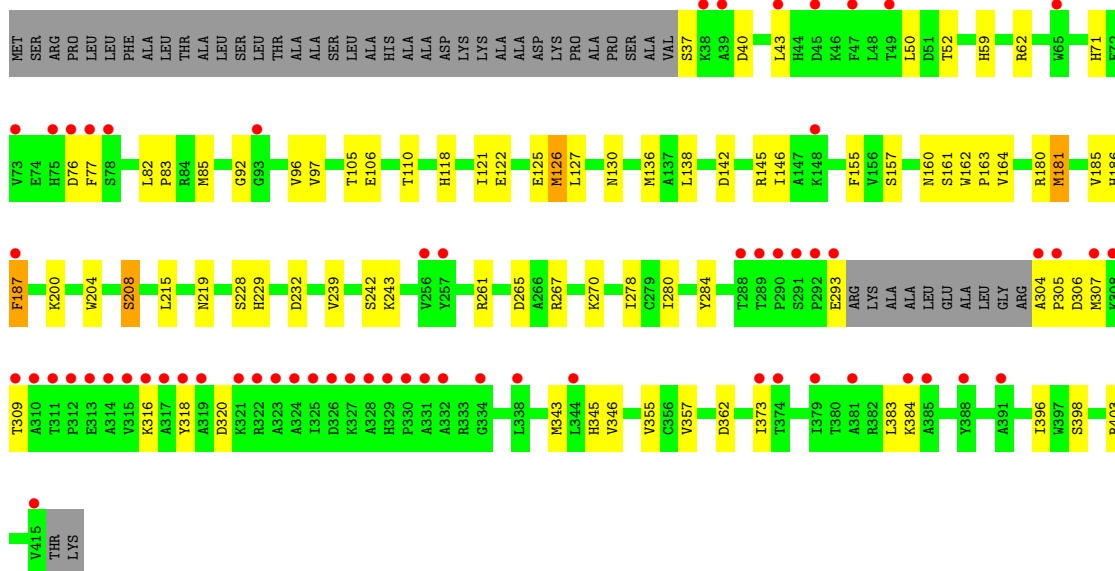
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	175	Total 175	O 175	0	0
4	B	156	Total 156	O 156	0	0
4	C	98	Total 98	O 98	0	0
4	D	95	Total 95	O 95	0	0



• Molecule 1: Dipeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.67Å 129.24Å 99.23Å 90.00° 104.76° 90.00°	Depositor
Resolution (Å)	24.98 – 2.00 24.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.3 (24.98-2.00) 92.3 (24.98-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 1.79Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.250 0.238 , 0.250	Depositor DCC
R_{free} test set	7877 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtrriage
Anisotropy	0.157	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11860	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	0.44	1/2896 (0.0%)	0.88	7/3926 (0.2%)
1	B	0.43	2/2896 (0.1%)	0.87	7/3926 (0.2%)
1	C	0.40	1/2896 (0.0%)	0.87	7/3926 (0.2%)
1	D	0.39	1/2896 (0.0%)	0.88	7/3926 (0.2%)
All	All	0.41	5/11584 (0.0%)	0.87	28/15704 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	MET	SD-CE	-7.49	1.60	1.79
1	B	181	MET	SD-CE	-6.41	1.63	1.79
1	D	181	MET	SD-CE	-6.07	1.64	1.79
1	C	181	MET	SD-CE	-5.71	1.65	1.79
1	B	126	MET	SD-CE	-5.66	1.65	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	VAL	N-CA-C	8.95	121.38	109.21
1	C	96	VAL	N-CA-C	8.92	121.34	109.21
1	A	96	VAL	N-CA-C	8.61	120.92	109.21
1	B	96	VAL	N-CA-C	8.61	120.91	109.21
1	A	280	ILE	N-CA-C	7.52	119.08	108.93
1	B	280	ILE	N-CA-C	7.41	118.94	108.93
1	D	280	ILE	N-CA-C	7.27	118.75	108.93
1	C	280	ILE	N-CA-C	7.23	118.69	108.93
1	A	155	PHE	N-CA-C	-6.00	101.64	110.52
1	C	155	PHE	N-CA-C	-5.71	102.07	110.52
1	D	155	PHE	N-CA-C	-5.58	102.26	110.52
1	C	357	VAL	N-CA-C	5.58	115.89	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	PHE	N-CA-C	5.55	118.26	111.82
1	A	97	VAL	N-CA-C	-5.54	98.98	106.85
1	B	155	PHE	N-CA-C	-5.53	102.34	110.52
1	C	97	VAL	N-CA-C	-5.46	99.09	106.85
1	D	357	VAL	N-CA-C	5.46	115.72	107.75
1	A	187	PHE	N-CA-C	5.37	118.05	111.82
1	A	357	VAL	N-CA-C	5.37	115.59	107.75
1	B	357	VAL	N-CA-C	5.36	115.58	107.75
1	D	97	VAL	N-CA-C	-5.30	99.32	106.85
1	B	97	VAL	N-CA-C	-5.29	99.34	106.85
1	B	208	SER	N-CA-C	-5.21	102.46	110.07
1	D	187	PHE	N-CA-C	5.17	117.82	111.82
1	D	208	SER	N-CA-C	-5.14	102.56	110.07
1	C	187	PHE	N-CA-C	5.13	117.77	111.82
1	A	208	SER	N-CA-C	-5.06	102.68	110.07
1	C	208	SER	N-CA-C	-5.04	102.72	110.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2831	0	2748	67	0
1	B	2831	0	2748	69	0
1	C	2831	0	2748	70	0
1	D	2831	0	2748	69	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	175	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	156	0	0	7	0
4	C	98	0	0	5	0
4	D	95	0	0	5	0
All	All	11860	0	10992	272	0

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 12.

All (272) 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:138:LEU:HB3	1:C:180:ARG:HH12	1.22	1.00
1:B:138:LEU:HB3	1:B:180:ARG:HH12	1.22	0.99
1:A:138:LEU:HB3	1:A:180:ARG:HH12	1.24	0.98
1:D:138:LEU:HB3	1:D:180:ARG:HH12	1.24	0.97
1:C:138:LEU:HB3	1:C:180:ARG:NH1	1.87	0.88
1:B:138:LEU:HB3	1:B:180:ARG:NH1	1.87	0.88
1:A:138:LEU:HB3	1:A:180:ARG:NH1	1.88	0.88
1:D:138:LEU:HB3	1:D:180:ARG:NH1	1.88	0.88
1:C:43:LEU:HD21	1:C:384:LYS:HG3	1.62	0.82
1:A:43:LEU:HD21	1:A:384:LYS:HG3	1.62	0.81
1:B:43:LEU:HD21	1:B:384:LYS:HG3	1.63	0.81
1:D:43:LEU:HD21	1:D:384:LYS:HG3	1.63	0.79
1:B:181:MET:HE3	4:B:475:HOH:O	1.82	0.77
1:A:306:ASP:HB3	1:A:309:THR:HG22	1.67	0.77
1:C:306:ASP:HB3	1:C:309:THR:HG22	1.67	0.76
1:B:306:ASP:HB3	1:B:309:THR:HG22	1.67	0.76
1:C:343:MET:HE2	1:C:383:LEU:HD21	1.68	0.75
1:D:306:ASP:HB3	1:D:309:THR:HG22	1.68	0.75
1:D:403:ARG:NH1	4:D:500:HOH:O	2.18	0.75
1:D:228:SER:O	1:D:229:HIS:HB2	1.88	0.73
1:D:343:MET:HE2	1:D:383:LEU:HD21	1.71	0.73
1:B:343:MET:HE2	1:B:383:LEU:HD21	1.71	0.72
1:D:126:MET:O	1:D:126:MET:HE2	1.89	0.72
1:A:343:MET:HE2	1:A:383:LEU:HD21	1.70	0.72
1:C:228:SER:O	1:C:229:HIS:HB2	1.90	0.72
1:D:181:MET:HE3	4:D:440:HOH:O	1.91	0.70
1:D:261:ARG:HG2	1:D:284:TYR:CD2	2.27	0.70
1:A:126:MET:O	1:A:126:MET:HE2	1.92	0.70
1:B:126:MET:HE2	1:B:126:MET:O	1.91	0.69
1:A:261:ARG:HG2	1:A:284:TYR:CD2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ARG:HG2	1:C:284:TYR:CD2	2.28	0.68
1:B:261:ARG:HG2	1:B:284:TYR:CD2	2.28	0.68
1:C:126:MET:HE2	1:C:126:MET:O	1.94	0.68
1:A:181:MET:HE3	4:A:427:HOH:O	1.95	0.67
1:A:228:SER:O	1:A:229:HIS:HB2	1.93	0.67
1:B:228:SER:O	1:B:229:HIS:HB2	1.94	0.66
1:D:71:HIS:HE1	4:D:468:HOH:O	1.77	0.66
1:B:329:HIS:HE1	4:B:556:HOH:O	1.78	0.65
1:C:181:MET:HE3	4:C:454:HOH:O	1.99	0.62
1:A:62:ARG:HG3	1:A:307:MET:O	2.00	0.62
1:B:52:THR:O	1:B:181:MET:HE1	2.00	0.62
1:A:219:ASN:HD21	1:A:242:SER:HA	1.64	0.61
1:B:343:MET:CE	1:B:396:ILE:HG21	2.30	0.61
1:C:180:ARG:NH1	4:C:501:HOH:O	2.33	0.61
1:B:110:THR:HG22	4:B:480:HOH:O	2.01	0.61
1:C:343:MET:HE1	1:C:383:LEU:HD11	1.83	0.60
1:B:343:MET:HE1	1:B:383:LEU:HD11	1.83	0.60
1:A:71:HIS:HE1	4:A:474:HOH:O	1.83	0.60
1:C:219:ASN:HD21	1:C:242:SER:HA	1.65	0.60
1:D:261:ARG:HG2	1:D:284:TYR:CE2	2.37	0.60
1:D:343:MET:CE	1:D:396:ILE:HG21	2.31	0.60
1:B:62:ARG:HG3	1:B:307:MET:O	2.02	0.60
1:A:343:MET:CE	1:A:396:ILE:HG21	2.32	0.60
1:C:82:LEU:HB3	1:C:83:PRO:HD3	1.84	0.59
1:B:126:MET:HE2	1:B:130:ASN:HD22	1.67	0.59
1:D:52:THR:O	1:D:181:MET:HE1	2.02	0.59
1:D:62:ARG:HG3	1:D:307:MET:O	2.01	0.59
1:D:219:ASN:HD21	1:D:242:SER:HA	1.67	0.59
1:C:62:ARG:HG3	1:C:307:MET:O	2.02	0.59
1:D:82:LEU:HB3	1:D:83:PRO:HD3	1.84	0.59
1:B:261:ARG:HG2	1:B:284:TYR:CE2	2.37	0.59
1:C:261:ARG:HG2	1:C:284:TYR:CE2	2.38	0.59
1:B:82:LEU:HB3	1:B:83:PRO:HD3	1.84	0.59
1:D:343:MET:HE1	1:D:383:LEU:HD11	1.84	0.59
1:A:343:MET:HE1	1:A:383:LEU:HD11	1.85	0.59
1:D:306:ASP:HB3	1:D:309:THR:CG2	2.33	0.58
1:B:219:ASN:HD21	1:B:242:SER:HA	1.67	0.58
1:C:343:MET:CE	1:C:396:ILE:HG21	2.33	0.58
1:A:219:ASN:ND2	1:A:243:LYS:H	2.02	0.58
1:A:306:ASP:HB3	1:A:309:THR:CG2	2.33	0.58
1:A:261:ARG:HG2	1:A:284:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ASP:HB3	1:B:309:THR:CG2	2.34	0.58
1:C:52:THR:O	1:C:181:MET:HE1	2.04	0.57
1:D:261:ARG:NH1	1:D:261:ARG:HG3	2.20	0.56
1:A:82:LEU:HB3	1:A:83:PRO:HD3	1.87	0.56
1:C:126:MET:HE2	1:C:130:ASN:HD22	1.70	0.56
1:D:59:HIS:HE1	1:D:362:ASP:OD1	1.88	0.56
1:D:126:MET:HE2	1:D:130:ASN:HD22	1.71	0.56
1:D:126:MET:CE	1:D:130:ASN:HB2	2.36	0.56
1:A:162:TRP:N	1:A:163:PRO:CD	2.69	0.55
1:A:126:MET:CE	1:A:130:ASN:HB2	2.36	0.55
1:A:126:MET:HE2	1:A:130:ASN:HD22	1.72	0.55
1:A:261:ARG:HG3	1:A:261:ARG:NH1	2.22	0.55
1:C:126:MET:CE	1:C:130:ASN:HB2	2.37	0.55
1:C:306:ASP:HB3	1:C:309:THR:CG2	2.34	0.55
1:A:52:THR:O	1:A:181:MET:HE1	2.06	0.55
1:D:261:ARG:HG3	1:D:261:ARG:HH11	1.72	0.55
1:C:59:HIS:HE1	1:C:362:ASP:OD1	1.89	0.55
1:D:186:HIS:CG	1:D:187:PHE:H	2.25	0.55
1:B:59:HIS:HE1	1:B:362:ASP:OD1	1.89	0.55
1:C:261:ARG:NH1	1:C:261:ARG:HG3	2.22	0.54
1:B:162:TRP:N	1:B:163:PRO:CD	2.70	0.54
1:D:110:THR:HG22	4:D:481:HOH:O	2.06	0.54
1:B:343:MET:HE3	1:B:396:ILE:HG21	1.88	0.54
1:D:343:MET:HE3	1:D:396:ILE:HG21	1.90	0.54
1:A:59:HIS:HE1	1:A:362:ASP:OD1	1.90	0.54
1:A:181:MET:CE	4:A:427:HOH:O	2.54	0.54
1:D:305:PRO:HD3	1:D:318:TYR:CG	2.43	0.54
1:A:50:LEU:HD12	1:A:50:LEU:C	2.33	0.54
1:C:50:LEU:HD12	1:C:50:LEU:C	2.32	0.54
1:C:157:SER:HB3	1:C:181:MET:HE2	1.90	0.54
1:C:265:ASP:OD1	1:C:345:HIS:HE1	1.91	0.54
1:B:126:MET:CE	1:B:130:ASN:HB2	2.38	0.54
1:A:76:ASP:O	1:A:77:PHE:HB2	2.07	0.54
1:B:261:ARG:NH1	1:B:261:ARG:HG3	2.22	0.53
1:D:76:ASP:O	1:D:77:PHE:HB2	2.08	0.53
1:D:162:TRP:N	1:D:163:PRO:CD	2.70	0.53
1:B:265:ASP:OD1	1:B:345:HIS:HE1	1.91	0.53
1:B:305:PRO:HD3	1:B:318:TYR:CG	2.43	0.53
1:D:50:LEU:C	1:D:50:LEU:HD12	2.34	0.53
1:A:186:HIS:CG	1:A:187:PHE:H	2.26	0.53
1:B:186:HIS:CG	1:B:187:PHE:H	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:HIS:CG	1:C:187:PHE:H	2.26	0.53
1:B:239:VAL:HG11	1:B:270:LYS:HG2	1.91	0.53
1:B:157:SER:HB3	1:B:181:MET:HE2	1.90	0.53
1:C:162:TRP:N	1:C:163:PRO:CD	2.71	0.53
1:D:265:ASP:OD1	1:D:345:HIS:HE1	1.91	0.53
1:A:239:VAL:HG11	1:A:270:LYS:HG2	1.90	0.53
1:B:219:ASN:ND2	1:B:243:LYS:H	2.06	0.53
1:D:121:ILE:O	1:D:125:GLU:HG3	2.09	0.52
1:D:346:VAL:HG12	1:D:355:VAL:HG22	1.91	0.52
1:A:265:ASP:OD1	1:A:345:HIS:HE1	1.92	0.52
1:C:76:ASP:O	1:C:77:PHE:HB2	2.08	0.52
1:C:71:HIS:HE1	4:C:474:HOH:O	1.92	0.52
1:C:261:ARG:HG3	1:C:261:ARG:HH11	1.73	0.52
1:A:305:PRO:HD3	1:A:318:TYR:CG	2.43	0.52
1:A:121:ILE:O	1:A:125:GLU:HG3	2.10	0.52
1:B:50:LEU:C	1:B:50:LEU:HD12	2.34	0.52
1:C:219:ASN:ND2	1:C:243:LYS:H	2.08	0.52
1:A:261:ARG:HG3	1:A:261:ARG:HH11	1.74	0.52
1:A:305:PRO:HD3	1:A:318:TYR:CD2	2.44	0.52
1:B:76:ASP:O	1:B:77:PHE:HB2	2.10	0.52
1:C:343:MET:HE3	1:C:396:ILE:HG21	1.90	0.52
1:D:239:VAL:HG11	1:D:270:LYS:HG2	1.91	0.52
1:B:305:PRO:HD3	1:B:318:TYR:CD2	2.44	0.52
1:C:239:VAL:HG11	1:C:270:LYS:HG2	1.92	0.52
1:C:346:VAL:HG12	1:C:355:VAL:HG22	1.91	0.52
1:D:305:PRO:HD3	1:D:318:TYR:CD2	2.44	0.52
1:C:157:SER:CB	1:C:181:MET:HE2	2.39	0.52
1:D:306:ASP:CB	1:D:309:THR:HG22	2.39	0.52
1:A:343:MET:HE3	1:A:396:ILE:HG21	1.92	0.51
1:C:305:PRO:HD3	1:C:318:TYR:CG	2.44	0.51
1:D:219:ASN:ND2	1:D:243:LYS:H	2.08	0.51
1:A:185:VAL:HG22	1:A:186:HIS:N	2.26	0.51
1:C:121:ILE:O	1:C:125:GLU:HG3	2.11	0.51
1:B:306:ASP:CB	1:B:309:THR:HG22	2.40	0.50
1:C:306:ASP:CB	1:C:309:THR:HG22	2.39	0.50
1:D:157:SER:HB3	1:D:181:MET:HE2	1.93	0.50
1:C:305:PRO:HD3	1:C:318:TYR:CD2	2.46	0.50
1:C:185:VAL:HG22	1:C:186:HIS:N	2.27	0.50
1:B:261:ARG:HG3	1:B:261:ARG:HH11	1.76	0.50
4:A:555:HOH:O	1:D:200:LYS:HG3	2.12	0.50
1:D:185:VAL:HG22	1:D:186:HIS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:VAL:HG22	1:B:186:HIS:N	2.27	0.50
1:B:346:VAL:HG12	1:B:355:VAL:HG22	1.93	0.50
1:A:346:VAL:HG12	1:A:355:VAL:HG22	1.93	0.49
1:B:71:HIS:HE1	4:B:441:HOH:O	1.94	0.49
1:A:306:ASP:CB	1:A:309:THR:HG22	2.39	0.49
1:B:293:GLU:CD	1:B:293:GLU:H	2.20	0.49
1:C:181:MET:CE	4:C:454:HOH:O	2.58	0.49
1:A:161:SER:C	1:A:163:PRO:HD2	2.37	0.48
1:A:293:GLU:CD	1:A:293:GLU:H	2.21	0.48
1:B:121:ILE:O	1:B:125:GLU:HG3	2.14	0.48
1:B:157:SER:CB	1:B:181:MET:HE2	2.44	0.48
1:A:157:SER:HB3	1:A:181:MET:HE2	1.96	0.47
1:D:37:SER:HB3	1:D:40:ASP:OD2	2.14	0.47
1:C:293:GLU:CD	1:C:293:GLU:H	2.21	0.47
1:B:106:GLU:O	1:B:110:THR:HG23	2.15	0.47
1:B:215:LEU:HD23	1:B:215:LEU:C	2.39	0.47
1:D:293:GLU:H	1:D:293:GLU:CD	2.22	0.47
1:A:157:SER:CB	1:A:181:MET:HE2	2.44	0.47
1:D:157:SER:CB	1:D:181:MET:HE2	2.45	0.47
1:C:215:LEU:C	1:C:215:LEU:HD23	2.40	0.47
1:C:106:GLU:O	1:C:110:THR:HG23	2.15	0.47
1:C:37:SER:HB3	1:C:40:ASP:OD2	2.16	0.46
1:D:106:GLU:O	1:D:110:THR:HG23	2.15	0.46
1:A:37:SER:HB3	1:A:40:ASP:OD2	2.16	0.46
1:A:180:ARG:HA	1:A:180:ARG:HD3	1.81	0.46
1:D:161:SER:C	1:D:163:PRO:HD2	2.41	0.45
1:D:215:LEU:HD23	1:D:215:LEU:C	2.41	0.45
1:C:343:MET:CE	1:C:383:LEU:HD21	2.44	0.45
1:D:186:HIS:CG	1:D:187:PHE:N	2.84	0.45
1:B:37:SER:HB3	1:B:40:ASP:OD2	2.17	0.45
1:B:203:ILE:HB	1:C:237:GLN:HG2	1.97	0.45
1:A:186:HIS:CG	1:A:187:PHE:N	2.84	0.45
1:A:389:SER:HB2	4:A:554:HOH:O	2.17	0.45
1:A:160:ASN:HB2	1:A:186:HIS:HB2	1.99	0.44
1:D:181:MET:CE	4:D:440:HOH:O	2.60	0.44
1:A:316:LYS:HG2	1:A:320:ASP:OD2	2.18	0.44
1:B:161:SER:C	1:B:163:PRO:HD2	2.42	0.44
1:A:50:LEU:HA	1:A:92:GLY:O	2.17	0.44
1:D:343:MET:HE1	1:D:396:ILE:HG21	1.99	0.44
1:B:50:LEU:HA	1:B:92:GLY:O	2.18	0.44
1:B:186:HIS:CG	1:B:187:PHE:N	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:CZ	1:A:307:MET:HE3	2.48	0.44
1:A:215:LEU:C	1:A:215:LEU:HD23	2.43	0.44
1:C:161:SER:C	1:C:163:PRO:HD2	2.42	0.44
1:A:204:TRP:CE2	1:A:208:SER:HB3	2.53	0.44
1:A:343:MET:HE1	1:A:396:ILE:HG21	1.99	0.44
1:C:50:LEU:HA	1:C:92:GLY:O	2.18	0.44
1:D:142:ASP:HA	1:D:145:ARG:NH1	2.33	0.44
1:B:107:LYS:HG3	4:B:460:HOH:O	2.17	0.43
1:C:142:ASP:HA	1:C:145:ARG:NH1	2.33	0.43
1:A:343:MET:CE	1:A:383:LEU:HD21	2.44	0.43
1:A:278:ILE:HD12	1:A:278:ILE:N	2.33	0.43
1:C:228:SER:O	1:C:229:HIS:CB	2.64	0.43
1:C:278:ILE:HD12	1:C:278:ILE:N	2.34	0.43
1:B:142:ASP:HA	1:B:145:ARG:NH1	2.34	0.43
1:C:62:ARG:CZ	1:C:307:MET:HE3	2.49	0.43
1:A:213:ARG:HG2	1:D:105:THR:HA	2.01	0.43
1:C:186:HIS:CG	1:C:187:PHE:N	2.85	0.43
1:C:316:LYS:HG2	1:C:320:ASP:OD2	2.19	0.43
1:C:142:ASP:O	1:C:146:ILE:HG13	2.18	0.43
1:B:181:MET:CE	4:B:475:HOH:O	2.52	0.43
1:A:204:TRP:CD2	1:A:208:SER:HB3	2.54	0.43
1:B:142:ASP:O	1:B:146:ILE:HG13	2.18	0.43
1:B:62:ARG:CZ	1:B:307:MET:HE3	2.49	0.43
1:B:161:SER:O	1:B:164:VAL:HG22	2.19	0.43
1:B:166:GLU:HG2	1:C:209:PRO:HB3	2.00	0.43
1:D:62:ARG:CZ	1:D:307:MET:HE3	2.49	0.43
1:D:118:HIS:O	1:D:122:GLU:HG3	2.18	0.43
1:D:161:SER:O	1:D:164:VAL:HG22	2.19	0.43
1:D:316:LYS:HG2	1:D:320:ASP:OD2	2.18	0.43
1:B:180:ARG:NH2	4:B:542:HOH:O	2.52	0.42
1:B:316:LYS:HG2	1:B:320:ASP:OD2	2.19	0.42
1:C:127:LEU:HD13	1:C:136:MET:HB2	2.00	0.42
1:D:278:ILE:N	1:D:278:ILE:HD12	2.34	0.42
1:D:142:ASP:O	1:D:146:ILE:HG13	2.20	0.42
1:D:304:ALA:HA	1:D:318:TYR:CD2	2.55	0.42
1:B:278:ILE:N	1:B:278:ILE:HD12	2.34	0.42
1:B:343:MET:CE	1:B:383:LEU:HD21	2.45	0.42
1:C:102:GLY:HA3	1:C:162:TRP:CH2	2.54	0.42
1:D:343:MET:CE	1:D:383:LEU:HD21	2.44	0.42
1:A:228:SER:O	1:A:229:HIS:CB	2.67	0.42
1:B:127:LEU:HD13	1:B:136:MET:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ASN:HB2	1:B:186:HIS:HB2	2.02	0.42
1:C:160:ASN:HB2	1:C:186:HIS:HB2	2.01	0.42
1:B:180:ARG:HA	1:B:180:ARG:HD3	1.82	0.42
1:B:304:ALA:HA	1:B:318:TYR:CD2	2.55	0.42
1:C:204:TRP:CD2	1:C:208:SER:HB3	2.55	0.42
1:A:106:GLU:O	1:A:110:THR:HG23	2.20	0.42
1:A:161:SER:C	1:A:163:PRO:CD	2.93	0.42
1:D:127:LEU:HD13	1:D:136:MET:HB2	2.01	0.42
1:B:343:MET:HE1	1:B:396:ILE:HG21	2.00	0.42
1:C:118:HIS:O	1:C:122:GLU:HG3	2.20	0.42
1:C:161:SER:O	1:C:164:VAL:HG22	2.19	0.42
1:C:204:TRP:CE2	1:C:208:SER:HB3	2.55	0.42
1:A:102:GLY:HA3	1:A:162:TRP:CH2	2.54	0.41
1:A:304:ALA:HA	1:A:318:TYR:CD2	2.55	0.41
1:A:340:MET:HG3	1:A:382:ARG:HG2	2.02	0.41
1:A:142:ASP:HA	1:A:145:ARG:NH1	2.35	0.41
1:A:142:ASP:O	1:A:146:ILE:HG13	2.19	0.41
1:C:126:MET:HE2	1:C:130:ASN:HB2	2.02	0.41
1:D:204:TRP:CD2	1:D:208:SER:HB3	2.55	0.41
1:D:50:LEU:HA	1:D:92:GLY:O	2.19	0.41
1:D:160:ASN:HB2	1:D:186:HIS:HB2	2.03	0.41
1:D:228:SER:O	1:D:229:HIS:CB	2.63	0.41
1:B:204:TRP:CD2	1:B:208:SER:HB3	2.54	0.41
1:D:85:MET:HA	1:D:373:ILE:HD12	2.03	0.41
1:A:118:HIS:O	1:A:122:GLU:HG3	2.21	0.41
1:B:232:ASP:HB3	1:B:267:ARG:CZ	2.51	0.41
1:B:198:ASP:HA	1:B:199:PRO:HD3	1.94	0.41
1:C:353:LYS:NZ	4:C:497:HOH:O	2.49	0.41
1:D:180:ARG:HA	1:D:180:ARG:HD3	1.82	0.41
1:C:232:ASP:HB3	1:C:267:ARG:CZ	2.51	0.41
1:C:321:LYS:O	1:C:325:ILE:HG13	2.20	0.41
1:A:161:SER:O	1:A:164:VAL:HG22	2.20	0.40
1:B:204:TRP:CE2	1:B:208:SER:HB3	2.56	0.40
1:D:126:MET:HE2	1:D:130:ASN:HB2	2.04	0.40
1:D:232:ASP:HB3	1:D:267:ARG:CZ	2.51	0.40
1:C:126:MET:HE1	1:C:134:PHE:CD2	2.56	0.40
1:C:376:LEU:N	1:C:377:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

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	365/417 (88%)	350 (96%)	14 (4%)	1 (0%)	36	35
1	B	365/417 (88%)	350 (96%)	14 (4%)	1 (0%)	36	35
1	C	365/417 (88%)	350 (96%)	14 (4%)	1 (0%)	36	35
1	D	365/417 (88%)	350 (96%)	14 (4%)	1 (0%)	36	35
All	All	1460/1668 (88%)	1400 (96%)	56 (4%)	4 (0%)	36	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	SER
1	B	398	SER
1	C	398	SER
1	D	398	SER

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	292/325 (90%)	290 (99%)	2 (1%)	76	82
1	B	292/325 (90%)	290 (99%)	2 (1%)	76	82
1	C	292/325 (90%)	291 (100%)	1 (0%)	86	91
1	D	292/325 (90%)	291 (100%)	1 (0%)	86	91
All	All	1168/1300 (90%)	1162 (100%)	6 (0%)	81	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	MET
1	A	293	GLU
1	B	126	MET
1	B	293	GLU
1	C	126	MET
1	D	126	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	70	HIS
1	A	86	ASN
1	A	130	ASN
1	A	205	ASN
1	A	219	ASN
1	A	345	HIS
1	B	59	HIS
1	B	70	HIS
1	B	71	HIS
1	B	86	ASN
1	B	118	HIS
1	B	130	ASN
1	B	219	ASN
1	B	345	HIS
1	C	59	HIS
1	C	70	HIS
1	C	86	ASN
1	C	130	ASN
1	C	219	ASN
1	C	329	HIS
1	C	345	HIS
1	D	59	HIS
1	D	70	HIS
1	D	86	ASN
1	D	130	ASN
1	D	219	ASN
1	D	345	HIS

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 12 ligands modelled in this entry, 12 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	369/417 (88%)	0.65	44 (11%) 9 8	23, 37, 63, 69	0
1	B	369/417 (88%)	0.81	53 (14%) 6 5	25, 41, 60, 67	0
1	C	369/417 (88%)	0.94	50 (13%) 7 6	28, 45, 64, 71	0
1	D	369/417 (88%)	1.07	62 (16%) 4 4	27, 46, 64, 71	0
All	All	1476/1668 (88%)	0.87	209 (14%) 6 5	23, 42, 63, 71	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	318	TYR	10.1
1	A	318	TYR	8.9
1	A	309	THR	6.9
1	A	64	GLY	6.9
1	D	315	VAL	6.5
1	A	314	ALA	6.5
1	C	318	TYR	6.3
1	D	292	PRO	6.3
1	D	318	TYR	6.1
1	A	77	PHE	6.0
1	A	304	ALA	5.7
1	D	304	ALA	5.5
1	D	325	ILE	5.4
1	B	293	GLU	5.3
1	A	329	HIS	5.3
1	A	305	PRO	5.2
1	A	310	ALA	5.1
1	A	311	THR	5.0
1	D	328	ALA	5.0
1	D	290	PRO	4.9
1	C	320	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	307	MET	4.8
1	C	330	PRO	4.7
1	D	324	ALA	4.7
1	C	293	GLU	4.6
1	C	329	HIS	4.6
1	A	187	PHE	4.6
1	A	312	PRO	4.6
1	C	312	PRO	4.6
1	A	315	VAL	4.5
1	C	292	PRO	4.5
1	D	305	PRO	4.5
1	B	46	LYS	4.5
1	A	325	ILE	4.4
1	D	314	ALA	4.3
1	C	315	VAL	4.3
1	D	323	ALA	4.2
1	B	77	PHE	4.2
1	C	328	ALA	4.1
1	A	317	ALA	4.1
1	C	325	ILE	4.1
1	C	291	SER	4.0
1	A	324	ALA	3.9
1	D	317	ALA	3.9
1	A	321	LYS	3.9
1	D	329	HIS	3.9
1	D	291	SER	3.9
1	D	77	PHE	3.9
1	A	328	ALA	3.8
1	D	326	ASP	3.8
1	B	315	VAL	3.8
1	A	148	LYS	3.8
1	C	74	GLU	3.8
1	D	321	LYS	3.8
1	C	311	THR	3.8
1	C	324	ALA	3.7
1	D	319	ALA	3.7
1	C	290	PRO	3.7
1	C	415	VAL	3.6
1	C	289	THR	3.6
1	B	64	GLY	3.6
1	B	291	SER	3.6
1	C	148	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	311	THR	3.6
1	B	327	LYS	3.6
1	C	316	LYS	3.5
1	D	148	LYS	3.4
1	A	306	ASP	3.4
1	D	313	GLU	3.3
1	D	388	TYR	3.3
1	D	78	SER	3.3
1	C	187	PHE	3.3
1	A	313	GLU	3.3
1	A	65	TRP	3.3
1	B	415	VAL	3.3
1	B	332	ALA	3.2
1	B	292	PRO	3.2
1	A	320	ASP	3.2
1	C	326	ASP	3.2
1	D	322	ARG	3.2
1	D	312	PRO	3.2
1	A	73	VAL	3.1
1	D	187	PHE	3.1
1	A	38	LYS	3.1
1	D	289	THR	3.1
1	B	314	ALA	3.1
1	C	39	ALA	3.1
1	D	43	LEU	3.1
1	D	330	PRO	3.1
1	C	61	GLY	3.1
1	A	292	PRO	3.1
1	D	310	ALA	3.1
1	C	332	ALA	3.0
1	B	63	PRO	3.0
1	D	316	LYS	3.0
1	B	39	ALA	3.0
1	D	338	LEU	3.0
1	D	332	ALA	3.0
1	D	73	VAL	3.0
1	A	319	ALA	2.9
1	B	385	ALA	2.9
1	C	331	ALA	2.9
1	A	327	LYS	2.9
1	C	317	ALA	2.9
1	B	73	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	288	THR	2.9
1	B	43	LEU	2.9
1	B	75	HIS	2.9
1	B	330	PRO	2.9
1	A	326	ASP	2.8
1	B	40	ASP	2.8
1	D	381	ALA	2.8
1	D	415	VAL	2.8
1	B	304	ALA	2.8
1	B	381	ALA	2.8
1	B	45	ASP	2.8
1	C	385	ALA	2.8
1	C	43	LEU	2.8
1	B	384	LYS	2.8
1	B	321	LYS	2.7
1	C	304	ALA	2.7
1	D	293	GLU	2.7
1	B	328	ALA	2.7
1	C	313	GLU	2.7
1	A	316	LYS	2.7
1	C	314	ALA	2.7
1	D	39	ALA	2.7
1	D	309	THR	2.7
1	C	319	ALA	2.6
1	B	47	PHE	2.6
1	C	374	THR	2.6
1	B	414	SER	2.6
1	A	415	VAL	2.6
1	C	327	LYS	2.6
1	D	344	LEU	2.6
1	D	379	ILE	2.6
1	B	353	LYS	2.6
1	B	413	LYS	2.6
1	A	381	ALA	2.6
1	C	323	ALA	2.6
1	A	290	PRO	2.6
1	A	330	PRO	2.6
1	D	256	VAL	2.5
1	C	46	LYS	2.5
1	A	255	ALA	2.5
1	B	331	ALA	2.5
1	D	331	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	391	ALA	2.5
1	C	75	HIS	2.5
1	D	75	HIS	2.5
1	B	62	ARG	2.5
1	D	45	ASP	2.5
1	B	316	LYS	2.5
1	D	308	LYS	2.5
1	C	336	PHE	2.4
1	B	368	ASP	2.4
1	C	256	VAL	2.4
1	C	305	PRO	2.4
1	C	338	LEU	2.4
1	D	76	ASP	2.4
1	A	37	SER	2.4
1	D	257	TYR	2.4
1	A	293	GLU	2.4
1	B	290	PRO	2.4
1	A	43	LEU	2.3
1	B	187	PHE	2.3
1	B	325	ILE	2.3
1	D	93	GLY	2.3
1	D	327	LYS	2.3
1	B	309	THR	2.3
1	C	287	ASP	2.3
1	D	334	GLY	2.3
1	D	307	MET	2.3
1	D	374	THR	2.2
1	C	384	LYS	2.2
1	B	42	ALA	2.2
1	B	37	SER	2.2
1	C	310	ALA	2.2
1	B	65	TRP	2.2
1	A	200	LYS	2.2
1	B	41	LYS	2.2
1	B	107	LYS	2.2
1	C	77	PHE	2.2
1	B	317	ALA	2.2
1	B	323	ALA	2.2
1	C	347	LEU	2.2
1	D	49	THR	2.2
1	C	73	VAL	2.1
1	A	331	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	385	ALA	2.1
1	D	38	LYS	2.1
1	D	384	LYS	2.1
1	B	387	GLY	2.1
1	C	62	ARG	2.1
1	A	107	LYS	2.1
1	B	38	LYS	2.1
1	A	332	ALA	2.1
1	B	72	GLU	2.1
1	B	329	HIS	2.1
1	B	382	ARG	2.1
1	D	47	PHE	2.1
1	B	344	LEU	2.0
1	C	59	HIS	2.0
1	D	373	ILE	2.0
1	D	65	TRP	2.0
1	A	205	ASN	2.0
1	C	306	ASP	2.0
1	B	289	THR	2.0
1	B	388	TYR	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(Å ²)	Q<0.9
3	CL	C	420	1/1	0.79	0.14	52,52,52,52	0
3	CL	B	420	1/1	0.80	0.17	50,50,50,50	0
3	CL	A	420	1/1	0.80	0.19	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	D	420	1/1	0.82	0.14	50,50,50,50	0
2	ZN	D	418	1/1	0.91	0.09	51,51,51,51	0
2	ZN	C	418	1/1	0.92	0.08	52,52,52,52	0
2	ZN	C	419	1/1	0.94	0.06	59,59,59,59	0
2	ZN	A	419	1/1	0.96	0.05	36,36,36,36	0
2	ZN	B	418	1/1	0.96	0.05	39,39,39,39	0
2	ZN	B	419	1/1	0.96	0.05	47,47,47,47	0
2	ZN	D	419	1/1	0.96	0.07	62,62,62,62	0
2	ZN	A	418	1/1	0.97	0.06	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.