



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:35 AM GMT

PDB ID : 2RAG
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
<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

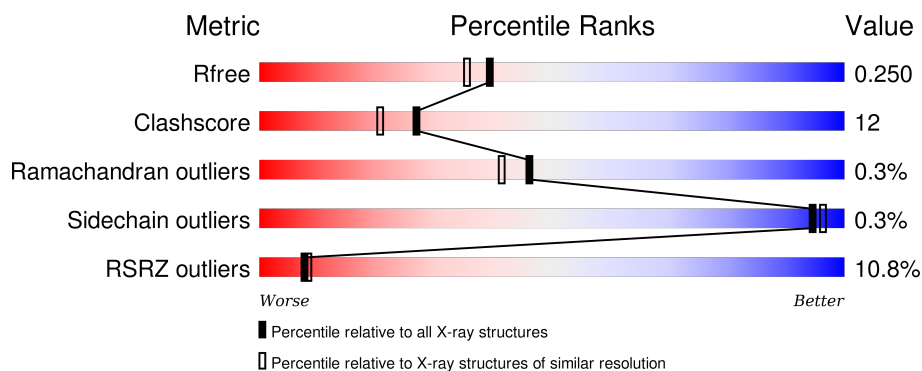
1 Overall quality at a glance

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	417	<div> <div>7%</div> <div>71% 17% 12%</div> </div>
1	B	417	<div> <div>4%</div> <div>70% 18% 12%</div> </div>
1	C	417	<div> <div>14%</div> <div>70% 19% 12%</div> </div>
1	D	417	<div> <div>13%</div> <div>70% 18% 12%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	420	-	-	-	X

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
1	A	369	Total	C	N	O	S	0	0	0
			2831	1783	492	545	11			
1	B	369	Total	C	N	O	S	0	0	0
			2831	1783	492	545	11			
1	C	369	Total	C	N	O	S	0	0	0
			2831	1783	492	545	11			
1	D	369	Total	C	N	O	S	0	0	0
			2831	1783	492	545	11			

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

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

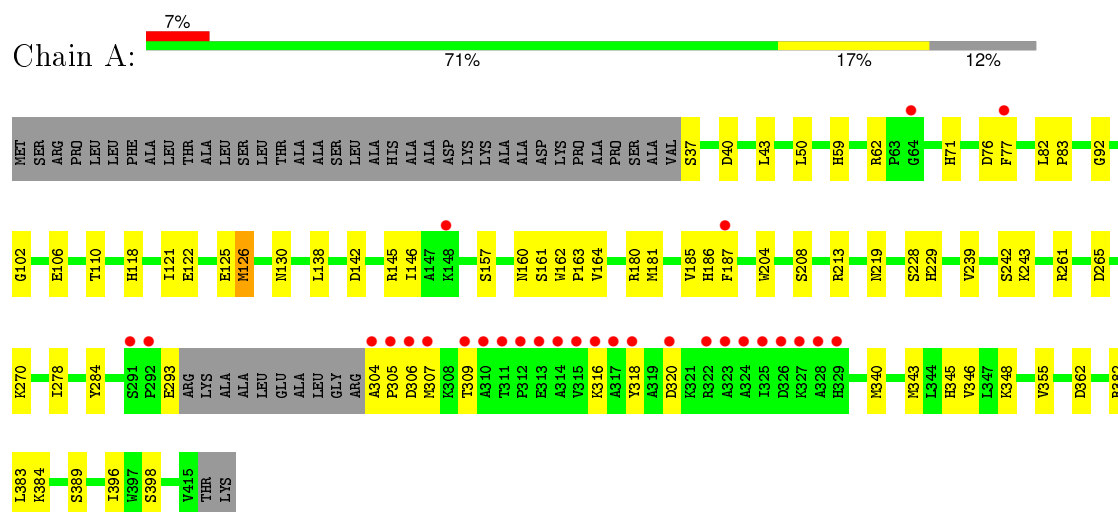
- Molecule 4 is water.

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

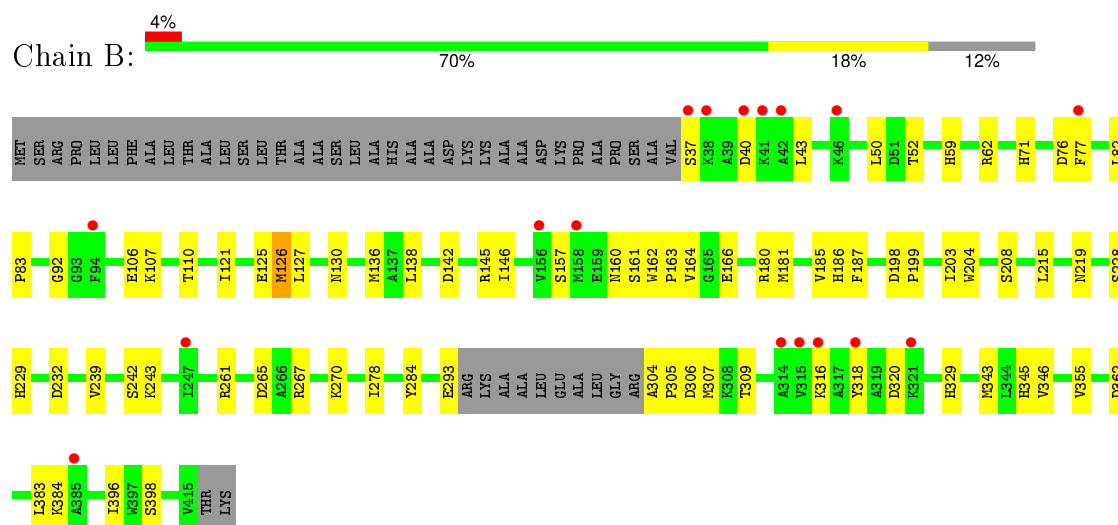
3 Residue-property plots

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Dipeptidase

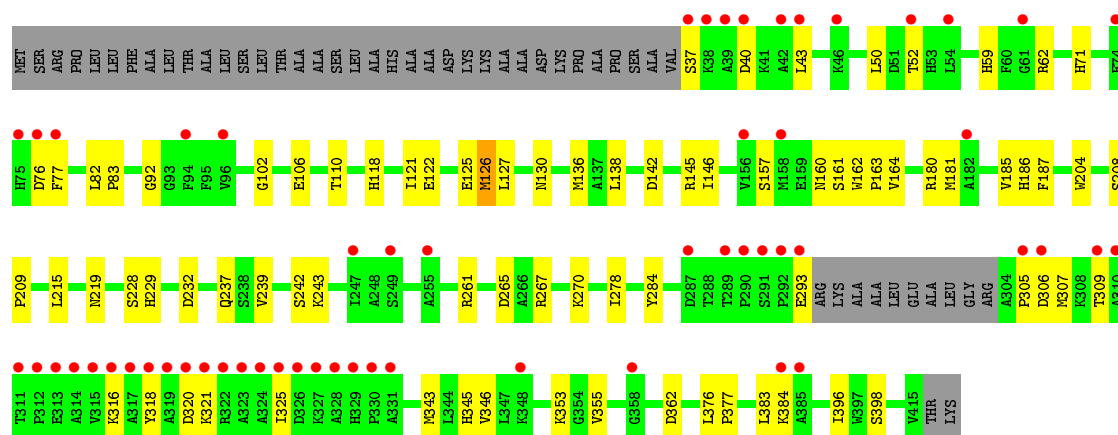


• Molecule 1: Dipeptidase

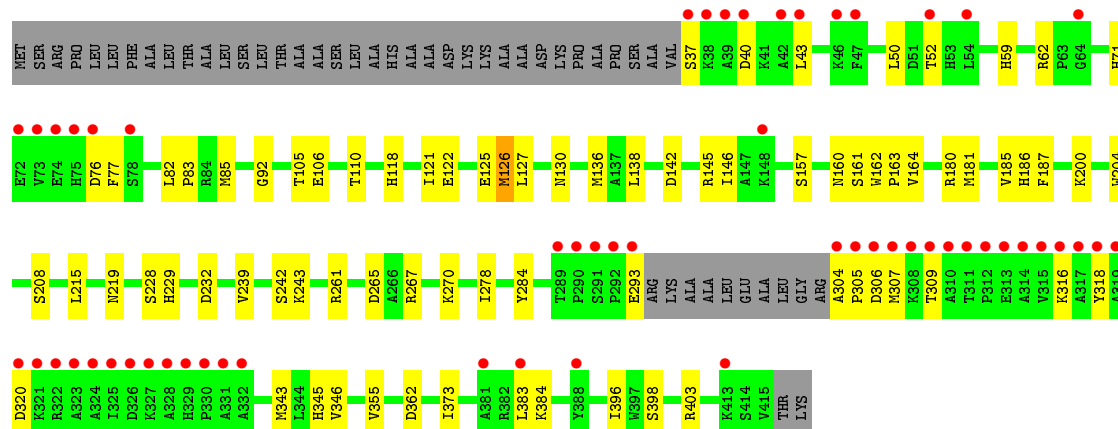


• Molecule 1: Dipeptidase





• 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 39.30 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (24.98-2.00) 78.2 (39.30-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.250 0.238 , 0.250	Depositor DCC
R_{free} test set	6124 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 156305 reflections	Xtriage
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

Xtriage'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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.35	0/2896	0.57	0/3926
1	B	0.34	0/2896	0.57	0/3926
1	C	0.33	0/2896	0.56	0/3926
1	D	0.33	0/2896	0.56	0/3926
All	All	0.34	0/11584	0.57	0/15704

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2831	0	2748	65	0
1	B	2831	0	2748	71	0
1	C	2831	0	2748	67	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	0
4	B	156	0	0	8	0
4	C	98	0	0	5	0
4	D	95	0	0	5	0
All	All	11860	0	10992	269	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 (269) 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: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:D:343:MET:HE2	1:D:383:LEU:HD21	1.69	0.75
1:B:126:MET:HE2	1:B:130:ASN:HD22	1.49	0.75
1:B:343:MET:HE2	1:B:383:LEU:HD21	1.69	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:A:126:MET:HE2	1:A:130:ASN:HD22	1.50	0.74
1:D:126:MET:HE2	1:D:130:ASN:HD22	1.51	0.74
1:C:343:MET:HE2	1:C:383:LEU:HD21	1.70	0.74
1:C:126:MET:HE2	1:C:130:ASN:HD22	1.51	0.74
1:D:228:SER:O	1:D:229:HIS:HB2	1.88	0.73
1:A:343:MET:HE2	1:A:383:LEU:HD21	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:SER:O	1:C:229:HIS:HB2	1.90	0.72
1:D:261:ARG:HG2	1:D:284:TYR:CD2	2.27	0.70
1:A:261:ARG:HG2	1:A:284:TYR:CD2	2.28	0.69
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:A:126:MET:HE2	1:A:130:ASN:ND2	2.08	0.67
1:A:228:SER:O	1:A:229:HIS:HB2	1.93	0.67
1:B:126:MET:HE2	1:B:130:ASN:ND2	2.10	0.66
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:126:MET:HE2	1:C:130:ASN:ND2	2.12	0.65
1:D:126:MET:HE2	1:D:126:MET:O	1.99	0.63
1:D:126:MET:HE2	1:D:130:ASN:ND2	2.14	0.63
1:A:62:ARG:HG3	1:A:307:MET:O	2.00	0.62
1:C:343:MET:HE1	1:C:383:LEU:HD11	1.82	0.61
1:B:343:MET:CE	1:B:396:ILE:HG21	2.30	0.61
1:A:219:ASN:HD21	1:A:242:SER:HA	1.64	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:219:ASN:HD21	1:C:242:SER:HA	1.65	0.60
1:A:71:HIS:HE1	4:A:474:HOH:O	1.83	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: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:C:261:ARG:HG2	1:C:284:TYR:CE2	2.38	0.59
1:B:261:ARG:HG2	1:B:284:TYR:CE2	2.37	0.59
1:B:82:LEU:HB3	1:B:83:PRO:HD3	1.84	0.59
1:B:343:MET:HE1	1:B:383:LEU:HD11	1.85	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:306:ASP:HB3	1:A:309:THR:CG2	2.33	0.58
1:B:126:MET:HE2	1:B:126:MET:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASN:ND2	1:A:243:LYS:H	2.02	0.58
1:A:261:ARG:HG2	1:A:284:TYR:CE2	2.38	0.58
1:B:306:ASP:HB3	1:B:309:THR:CG2	2.34	0.58
1:D:343:MET:HE1	1:D:383:LEU:HD11	1.86	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:B:181:MET:CE	4:B:475:HOH:O	2.52	0.56
1:D:59:HIS:HE1	1:D:362:ASP:OD1	1.88	0.56
1:D:126:MET:CE	1:D:130:ASN:HB2	2.36	0.56
1:B:157:SER:HB2	1:B:181:MET:HE3	1.88	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:C:306:ASP:HB3	1:C:309:THR:CG2	2.34	0.55
1:C:126:MET:CE	1:C:130:ASN:HB2	2.37	0.55
1:A:261:ARG:NH1	1:A:261:ARG:HG3	2.22	0.55
1:D:261:ARG:HH11	1:D:261:ARG:HG3	1.72	0.55
1:C:59:HIS:HE1	1:C:362:ASP:OD1	1.89	0.55
1:C:126:MET:HE2	1:C:126:MET:O	2.06	0.55
1:B:181:MET:HE1	4:B:475:HOH:O	2.05	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:157:SER:HB2	1:C:181:MET:HE3	1.88	0.55
1:C:261:ARG:HG3	1:C:261:ARG:NH1	2.22	0.54
1:D:110:THR:HG22	4:D:481:HOH:O	2.06	0.54
1:B:162:TRP:N	1:B:163:PRO:CD	2.70	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: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:C:343:MET:HE3	1:C:396:ILE:HG21	1.89	0.53
1:B:186:HIS:CG	1:B:187:PHE:H	2.26	0.53
1:C:186:HIS:CG	1:C:187:PHE:H	2.26	0.53
1:D:157:SER:HB2	1:D:181:MET:HE3	1.91	0.53
1:A:186:HIS:CG	1:A:187:PHE:H	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:VAL:HG11	1:B:270:LYS:HG2	1.91	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:B:219:ASN:ND2	1:B:243:LYS:H	2.06	0.53
1:A:239:VAL:HG11	1:A:270:LYS:HG2	1.90	0.53
1:D:346:VAL:HG12	1:D:355:VAL:HG22	1.91	0.52
1:D:121:ILE:O	1:D:125:GLU:HG3	2.09	0.52
1:C:76:ASP:O	1:C:77:PHE:HB2	2.08	0.52
1:A:265:ASP:OD1	1:A:345:HIS:HE1	1.92	0.52
1:C:261:ARG:HG3	1:C:261:ARG:HH11	1.73	0.52
1:C:71:HIS:HE1	4:C:474:HOH:O	1.92	0.52
1:A:305:PRO:HD3	1:A:318:TYR:CG	2.43	0.52
1:B:343:MET:HE3	1:B:396:ILE:HG21	1.90	0.52
1:C:219:ASN:ND2	1:C:243:LYS:H	2.08	0.52
1:A:181:MET:HE3	4:A:427:HOH:O	2.07	0.52
1:A:121:ILE:O	1:A:125:GLU:HG3	2.10	0.52
1:D:343:MET:HE3	1:D:396:ILE:HG21	1.92	0.52
1:A:261:ARG:HH11	1:A:261:ARG:HG3	1.74	0.52
1:C:181:MET:CE	4:C:454:HOH:O	2.58	0.52
1:A:305:PRO:HD3	1:A:318:TYR:CD2	2.44	0.52
1:D:239:VAL:HG11	1:D:270:LYS:HG2	1.91	0.52
1:B:76:ASP:O	1:B:77:PHE:HB2	2.10	0.52
1:A:157:SER:HB2	1:A:181:MET:HE2	1.92	0.52
1:D:305:PRO:HD3	1:D:318:TYR:CD2	2.44	0.52
1:B:305:PRO:HD3	1:B:318:TYR:CD2	2.44	0.52
1:C:346:VAL:HG12	1:C:355:VAL:HG22	1.91	0.52
1:C:239:VAL:HG11	1:C:270:LYS:HG2	1.92	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:C:181:MET:HE1	4:C:454:HOH:O	2.11	0.51
1:C:306:ASP:CB	1:C:309:THR:HG22	2.39	0.50
1:B:306:ASP:CB	1:B:309:THR:HG22	2.40	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:D:181:MET:CE	4:D:440:HOH:O	2.60	0.50
1:B:261:ARG:HG3	1:B:261:ARG:HH11	1.76	0.50
1:D:185:VAL:HG22	1:D:186:HIS:N	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:555:HOH:O	1:D:200:LYS:HG3	2.12	0.50
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:C:50:LEU:C	1:C:50:LEU:HD12	2.32	0.49
1:B:71:HIS:HE1	4:B:441:HOH:O	1.94	0.49
1:A:50:LEU:C	1:A:50:LEU:HD12	2.33	0.49
1:A:126:MET:HE2	1:A:126:MET:O	2.13	0.49
1:A:306:ASP:CB	1:A:309:THR:HG22	2.39	0.49
1:D:50:LEU:HD12	1:D:50:LEU:C	2.34	0.48
1:B:52:THR:O	1:B:181:MET:HE1	2.13	0.48
1:B:121:ILE:O	1:B:125:GLU:HG3	2.14	0.48
1:B:50:LEU:C	1:B:50:LEU:HD12	2.34	0.47
1:D:37:SER:HB3	1:D:40:ASP:OD2	2.14	0.47
1:B:106:GLU:O	1:B:110:THR:HG23	2.15	0.47
1:C:106:GLU:O	1:C:110:THR:HG23	2.15	0.47
1:A:126:MET:HE1	1:A:130:ASN:HB2	1.96	0.46
1:C:37:SER:HB3	1:C:40:ASP:OD2	2.16	0.46
1:D:343:MET:HE1	1:D:396:ILE:HG21	1.97	0.46
1:D:106:GLU:O	1:D:110:THR:HG23	2.15	0.46
1:A:180:ARG:HD3	1:A:180:ARG:HA	1.81	0.46
1:B:157:SER:CB	1:B:181:MET:HE3	2.46	0.46
1:A:37:SER:HB3	1:A:40:ASP:OD2	2.16	0.46
1:D:52:THR:O	1:D:181:MET:HE1	2.15	0.46
1:B:186:HIS:CG	1:B:187:PHE:N	2.84	0.45
1:C:343:MET:CE	1:C:383:LEU:HD21	2.44	0.45
1:B:293:GLU:H	1:B:293:GLU:CD	2.20	0.45
1:D:186:HIS:CG	1:D:187:PHE:N	2.84	0.45
1:D:181:MET:HE1	4:D:440:HOH:O	2.17	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:A:316:LYS:HG2	1:A:320:ASP:OD2	2.18	0.44
1:A:50:LEU:HA	1:A:92:GLY:O	2.17	0.44
1:B:50:LEU:HA	1:B:92:GLY:O	2.18	0.44
1:B:343:MET:HE1	1:B:396:ILE:HG21	1.98	0.44
1:A:293:GLU:H	1:A:293:GLU:CD	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ASP:HA	1:D:145:ARG:NH1	2.33	0.44
1:A:204:TRP:CE2	1:A:208:SER:HB3	2.53	0.44
1:A:161:SER:C	1:A:163:PRO:HD2	2.37	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:C:228:SER:O	1:C:229:HIS:CB	2.64	0.43
1:A:278:ILE:HD12	1:A:278:ILE:N	2.33	0.43
1:C:278:ILE:HD12	1:C:278:ILE:N	2.34	0.43
1:B:215:LEU:HD23	1:B:215:LEU:C	2.39	0.43
1:B:142:ASP:HA	1:B:145:ARG:NH1	2.34	0.43
1:C:186:HIS:CG	1:C:187:PHE:N	2.85	0.43
1:A:213:ARG:HG2	1:D:105:THR:HA	2.01	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: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:161:SER:O	1:B:164:VAL:HG22	2.19	0.43
1:D:161:SER:O	1:D:164:VAL:HG22	2.19	0.43
1:B:166:GLU:HG2	1:C:209:PRO:HB3	2.00	0.43
1:D:118:HIS:O	1:D:122:GLU:HG3	2.18	0.43
1:D:316:LYS:HG2	1:D:320:ASP:OD2	2.18	0.43
1:C:52:THR:O	1:C:181:MET:HE1	2.19	0.42
1:B:180:ARG:NH2	4:B:542:HOH:O	2.52	0.42
1:B:126:MET:HE1	1:B:130:ASN:HB2	2.01	0.42
1:D:278:ILE:HD12	1:D:278:ILE:N	2.34	0.42
1:D:293:GLU:H	1:D:293:GLU:CD	2.22	0.42
1:C:127:LEU:HD13	1:C:136:MET:HB2	2.00	0.42
1:B:316:LYS:HG2	1:B:320:ASP:OD2	2.19	0.42
1:D:304:ALA:HA	1:D:318:TYR:CD2	2.55	0.42
1:D:142:ASP:O	1:D:146:ILE:HG13	2.20	0.42
1:B:343:MET:CE	1:B:383:LEU:HD21	2.45	0.42
1:B:278:ILE:N	1:B:278:ILE:HD12	2.34	0.42
1:D:343:MET:CE	1:D:383:LEU:HD21	2.44	0.42
1:C:102:GLY:HA3	1:C:162:TRP:CH2	2.54	0.42
1:A:228:SER:O	1:A:229:HIS:CB	2.67	0.42
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:C:293:GLU:H	1:C:293:GLU:CD	2.21	0.42
1:C:215:LEU:C	1:C:215:LEU:HD23	2.40	0.42
1:B:127:LEU:HD13	1:B:136:MET:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:127:LEU:HD13	1:D:136:MET:HB2	2.01	0.42
1:A:106:GLU:O	1:A:110:THR:HG23	2.20	0.42
1:C:204:TRP:CE2	1:C:208:SER:HB3	2.55	0.42
1:C:161:SER:O	1:C:164:VAL:HG22	2.19	0.42
1:C:118:HIS:O	1:C:122:GLU:HG3	2.20	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:O	1:A:146:ILE:HG13	2.19	0.41
1:A:142:ASP:HA	1:A:145:ARG:NH1	2.35	0.41
1:D:204:TRP:CD2	1:D:208:SER:HB3	2.55	0.41
1:D:228:SER:O	1:D:229:HIS:CB	2.63	0.41
1:D:160:ASN:HB2	1:D:186:HIS:HB2	2.03	0.41
1:D:50:LEU:HA	1:D:92:GLY:O	2.19	0.41
1:D:157:SER:CB	1:D:181:MET:HE3	2.50	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:D:180:ARG:HD3	1:D:180:ARG:HA	1.82	0.41
1:C:353:LYS:NZ	4:C:497:HOH:O	2.49	0.41
1:B:198:ASP:HA	1:B:199:PRO:HD3	1.94	0.41
1:C:126:MET:HE1	1:C:130:ASN:HB2	2.03	0.41
1:D:161:SER:C	1:D:163:PRO:HD2	2.41	0.41
1:C:321:LYS:O	1:C:325:ILE:HG13	2.20	0.41
1:C:232:ASP:HB3	1:C:267:ARG:CZ	2.51	0.41
1:D:215:LEU:C	1:D:215:LEU:HD23	2.41	0.41
1:D:126:MET:HE1	1:D:130:ASN:HB2	2.03	0.40
1:B:181:MET:HE3	4:B:475:HOH:O	2.20	0.40
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:232:ASP:HB3	1:D:267:ARG:CZ	2.51	0.40
1:B:161:SER:C	1:B:163:PRO:HD2	2.42	0.40
1:A:348:LYS:NZ	4:A:580:HOH:O	2.52	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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/417 (88%)	350 (96%)	14 (4%)	1 (0%)	46	41
1	B	365/417 (88%)	350 (96%)	14 (4%)	1 (0%)	46	41
1	C	365/417 (88%)	350 (96%)	14 (4%)	1 (0%)	46	41
1	D	365/417 (88%)	350 (96%)	14 (4%)	1 (0%)	46	41
All	All	1460/1668 (88%)	1400 (96%)	56 (4%)	4 (0%)	46	41

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 ⓘ

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%)	291 (100%)	1 (0%)	94	96
1	B	292/325 (90%)	291 (100%)	1 (0%)	94	96
1	C	292/325 (90%)	291 (100%)	1 (0%)	94	96
1	D	292/325 (90%)	291 (100%)	1 (0%)	94	96
All	All	1168/1300 (90%)	1164 (100%)	4 (0%)	94	96

All (4) residues with a non-rotameric sidechain are listed below:

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) 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	219	ASN
1	A	345	HIS
1	B	59	HIS
1	B	70	HIS
1	B	71	HIS
1	B	86	ASN
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	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 ⓘ

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 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%)	0.24	29 (7%) 15 16	23, 37, 63, 69	0
1	B	369/417 (88%)	0.17	17 (4%) 36 38	25, 41, 60, 67	0
1	C	369/417 (88%)	0.66	57 (15%) 3 3	28, 45, 64, 71	0
1	D	369/417 (88%)	0.80	56 (15%) 3 3	27, 46, 64, 71	0
All	All	1476/1668 (88%)	0.47	159 (10%) 8 8	23, 42, 63, 71	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	315	VAL	10.2
1	D	318	TYR	9.9
1	B	318	TYR	9.3
1	D	292	PRO	9.3
1	C	318	TYR	8.9
1	D	310	ALA	8.6
1	A	318	TYR	8.5
1	C	312	PRO	8.2
1	C	315	VAL	7.9
1	A	309	THR	7.7
1	D	329	HIS	7.7
1	D	313	GLU	7.7
1	D	311	THR	7.6
1	D	325	ILE	7.5
1	A	314	ALA	7.1
1	C	330	PRO	7.1
1	C	311	THR	7.0
1	C	316	LYS	7.0
1	A	329	HIS	6.7
1	A	310	ALA	6.7
1	D	305	PRO	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	304	ALA	6.4
1	D	322	ARG	6.2
1	D	319	ALA	6.2
1	D	316	LYS	6.1
1	A	307	MET	6.1
1	A	325	ILE	6.0
1	D	321	LYS	5.9
1	C	320	ASP	5.9
1	D	314	ALA	5.8
1	D	312	PRO	5.7
1	A	305	PRO	5.6
1	A	313	GLU	5.4
1	A	312	PRO	5.4
1	D	326	ASP	5.3
1	C	313	GLU	5.3
1	C	291	SER	5.2
1	A	317	ALA	5.2
1	C	319	ALA	5.2
1	C	289	THR	5.1
1	A	311	THR	5.0
1	C	292	PRO	5.0
1	A	77	PHE	5.0
1	C	317	ALA	5.0
1	D	328	ALA	4.9
1	D	291	SER	4.9
1	D	290	PRO	4.9
1	C	328	ALA	4.8
1	D	327	LYS	4.8
1	D	38	LYS	4.8
1	C	326	ASP	4.7
1	A	328	ALA	4.6
1	A	292	PRO	4.5
1	D	309	THR	4.5
1	A	327	LYS	4.5
1	D	75	HIS	4.5
1	D	330	PRO	4.3
1	C	329	HIS	4.3
1	C	327	LYS	4.2
1	B	46	LYS	4.2
1	D	39	ALA	4.1
1	C	74	GLU	4.1
1	A	304	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	38	LYS	4.1
1	C	310	ALA	4.0
1	A	324	ALA	4.0
1	C	309	THR	4.0
1	C	324	ALA	3.9
1	C	42	ALA	3.9
1	C	323	ALA	3.9
1	A	64	GLY	3.9
1	A	306	ASP	3.8
1	D	320	ASP	3.8
1	A	316	LYS	3.8
1	B	38	LYS	3.8
1	D	293	GLU	3.8
1	D	332	ALA	3.7
1	B	40	ASP	3.7
1	C	37	SER	3.5
1	C	293	GLU	3.5
1	C	96	VAL	3.5
1	D	307	MET	3.5
1	D	317	ALA	3.5
1	D	43	LEU	3.5
1	C	43	LEU	3.4
1	D	64	GLY	3.4
1	D	324	ALA	3.4
1	B	37	SER	3.4
1	D	289	THR	3.3
1	D	74	GLU	3.3
1	A	148	LYS	3.3
1	D	308	LYS	3.2
1	D	42	ALA	3.1
1	B	41	LYS	3.1
1	C	325	ILE	3.1
1	C	46	LYS	3.1
1	D	148	LYS	3.1
1	D	306	ASP	3.1
1	A	315	VAL	3.0
1	C	305	PRO	3.0
1	D	46	LYS	3.0
1	A	291	SER	3.0
1	C	249	SER	3.0
1	C	156	VAL	3.0
1	C	54	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	75	HIS	3.0
1	C	287	ASP	2.9
1	C	39	ALA	2.9
1	B	316	LYS	2.9
1	D	40	ASP	2.8
1	B	315	VAL	2.8
1	D	37	SER	2.8
1	C	306	ASP	2.7
1	A	323	ALA	2.7
1	D	54	LEU	2.7
1	B	247	ILE	2.7
1	D	388	TYR	2.7
1	C	40	ASP	2.7
1	C	322	ARG	2.7
1	B	321	LYS	2.6
1	C	331	ALA	2.6
1	C	314	ALA	2.6
1	C	52	THR	2.5
1	C	321	LYS	2.5
1	A	322	ARG	2.5
1	B	385	ALA	2.5
1	C	384	LYS	2.4
1	C	385	ALA	2.4
1	D	76	ASP	2.4
1	A	326	ASP	2.4
1	C	348	LYS	2.4
1	D	47	PHE	2.4
1	B	314	ALA	2.4
1	C	290	PRO	2.4
1	A	320	ASP	2.3
1	A	187	PHE	2.3
1	B	94	PHE	2.3
1	B	156	VAL	2.2
1	C	247	ILE	2.2
1	D	381	ALA	2.2
1	D	323	ALA	2.2
1	B	77	PHE	2.2
1	C	61	GLY	2.1
1	D	72	GLU	2.1
1	C	77	PHE	2.1
1	C	94	PHE	2.1
1	C	182	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	255	ALA	2.1
1	C	358	GLY	2.1
1	D	413	LYS	2.1
1	D	383	LEU	2.1
1	B	158	MET	2.1
1	D	73	VAL	2.1
1	D	52	THR	2.0
1	B	42	ALA	2.0
1	C	158	MET	2.0
1	D	331	ALA	2.0
1	C	76	ASP	2.0
1	D	78	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CL	B	420	1/1	0.62	0.17	2.09	50,50,50,50	0
3	CL	A	420	1/1	0.63	0.17	1.46	52,52,52,52	0
3	CL	D	420	1/1	0.57	0.17	0.52	50,50,50,50	0
2	ZN	D	419	1/1	0.92	0.16	-0.45	62,62,62,62	0
3	CL	C	420	1/1	0.85	0.13	-0.59	52,52,52,52	0
2	ZN	C	419	1/1	0.94	0.12	-0.59	59,59,59,59	0
2	ZN	C	418	1/1	0.88	0.11	-1.14	52,52,52,52	0
2	ZN	B	419	1/1	0.92	0.11	-1.44	47,47,47,47	0
2	ZN	D	418	1/1	0.82	0.09	-1.74	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	A	418	1/1	0.99	0.06	-1.97	36,36,36,36	0
2	ZN	A	419	1/1	0.99	0.04	-2.57	36,36,36,36	0
2	ZN	B	418	1/1	0.97	0.07	-3.01	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.