



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:30 AM UTC

PDB ID : 1W7V / pdb_00001w7v
Title : ZnMg substituted aminopeptidase P from E. coli
Authors : Graham, S.C.; Bond, C.S.; Freeman, H.C.; Guss, J.M.
Deposited on : 2004-09-13
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
Mogul	:	2022.3.0, CSD as543be (2022)
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

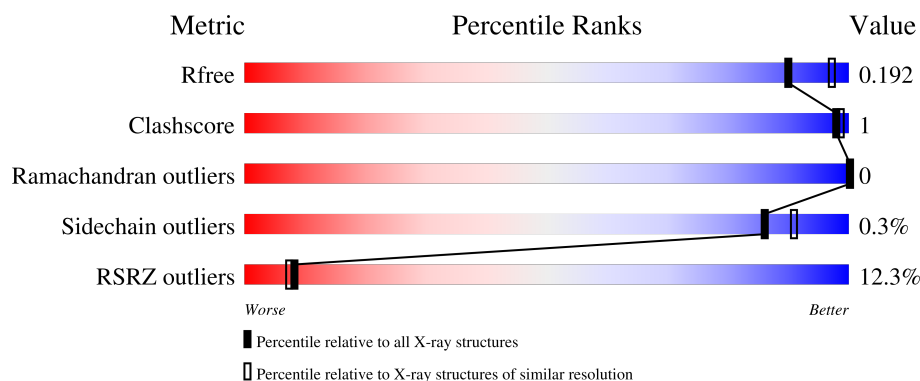
1 Overall quality at a glance

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	440	8% 97%
1	B	440	5% 98%
1	C	440	27% 97%
1	D	440	8% 97%
2	E	3	67% 67% 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	3	67% 33%
2	G	3	67% 33%
2	H	3	67% 33%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15192 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 XAA-PRO AMINOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	1	1
			3500	2201	620	664	15			
1	B	439	Total	C	N	O	S	0	4	0
			3512	2207	624	666	15			
1	C	439	Total	C	N	O	S	0	3	0
			3508	2205	624	664	15			
1	D	439	Total	C	N	O	S	0	2	0
			3500	2201	618	666	15			

- Molecule 2 is a protein called PEPTIDE VAL-PRO-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			16	11	2	3			
2	F	2	Total	C	N	O	0	0	0
			16	11	2	3			
2	G	2	Total	C	N	O	0	0	0
			16	11	2	3			
2	H	2	Total	C	N	O	0	0	0
			16	11	2	3			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	2	Total 2	Mg 2	0	0
4	C	1	Total 1	Mg 1	0	0
4	D	2	Total 2	Mg 2	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

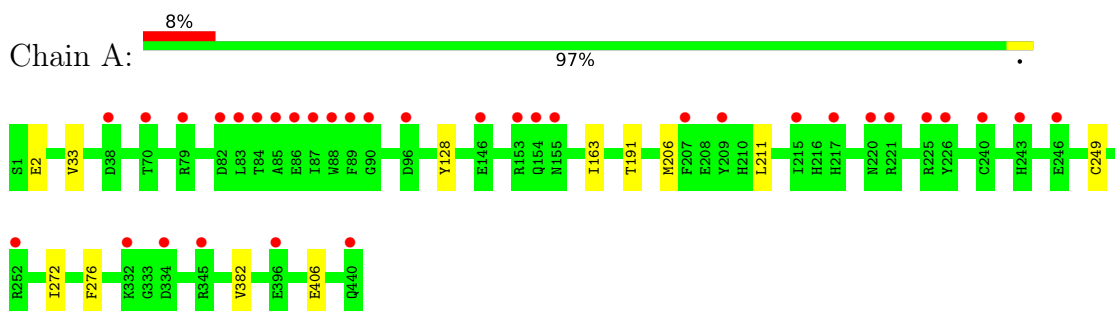
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	270	Total 270	O 270	0	0
6	B	344	Total 344	O 344	0	0
6	C	137	Total 137	O 137	0	2
6	D	337	Total 337	O 337	0	0
6	E	2	Total 2	O 2	0	0
6	F	2	Total 2	O 2	0	0
6	H	2	Total 2	O 2	0	0

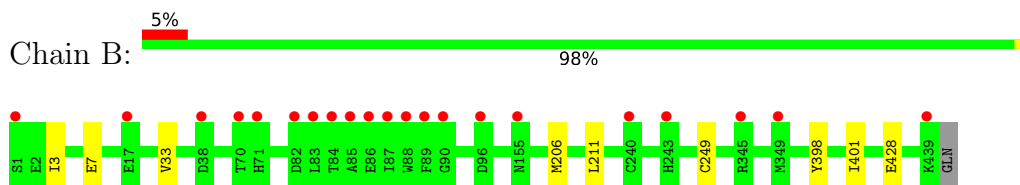
3 Residue-property plots [i](#)

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.

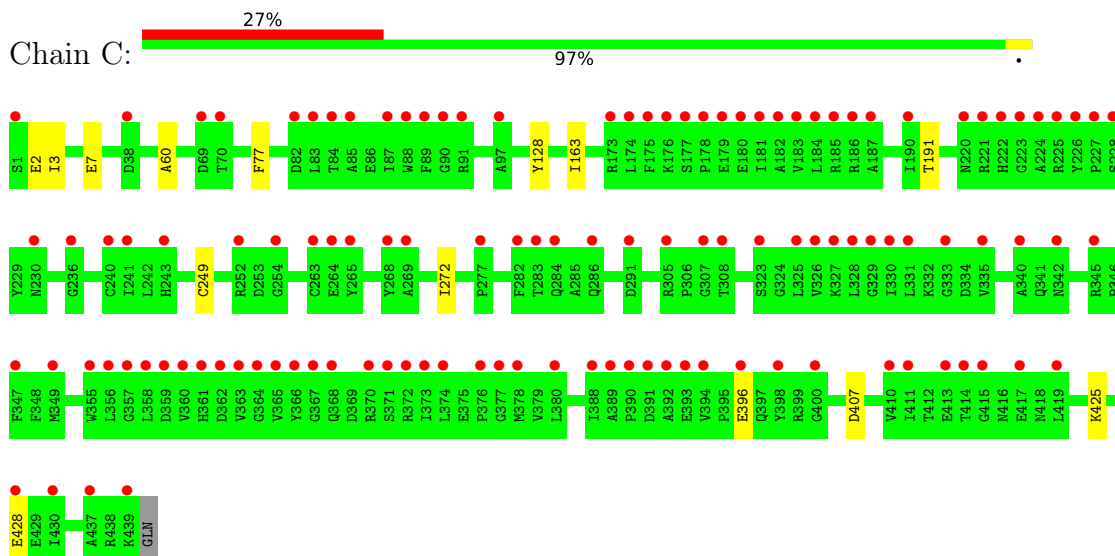
• Molecule 1: XAA-PRO AMINOPEPTIDASE



• Molecule 1: XAA-PRO AMINOPEPTIDASE

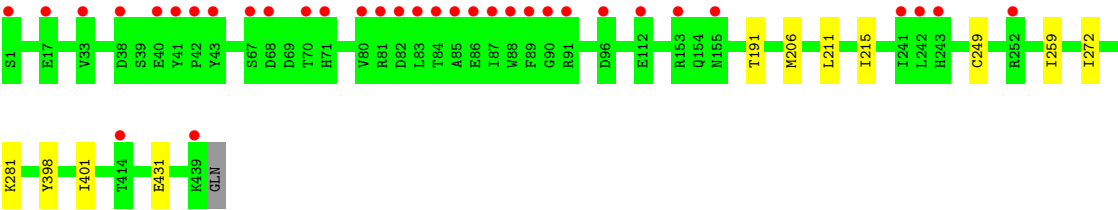


• Molecule 1: XAA-PRO AMINOPEPTIDASE



• Molecule 1: XAA-PRO AMINOPEPTIDASE





• Molecule 2: PEPTIDE VAL-PRO-LEU



• Molecule 2: PEPTIDE VAL-PRO-LEU



• Molecule 2: PEPTIDE VAL-PRO-LEU



• Molecule 2: PEPTIDE VAL-PRO-LEU



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.73Å 236.53Å 138.00Å 90.00° 106.34° 90.00°	Depositor
Resolution (Å)	37.80 – 2.00 37.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (37.80-2.00) 97.9 (37.80-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.156 , 0.180 0.169 , 0.192	Depositor DCC
R_{free} test set	11297 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15192	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: OCS, MG, 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	0.57	0/3567	0.68	1/4829 (0.0%)
1	B	0.60	0/3594	0.71	0/4864
1	C	0.52	0/3585	0.70	0/4852
1	D	0.60	0/3572	0.71	0/4836
2	E	0.30	0/16	0.61	0/19
2	F	0.37	0/16	0.65	0/19
2	G	0.23	0/16	0.57	0/19
2	H	0.25	0/16	0.55	0/19
All	All	0.57	0/14382	0.70	1/19457 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	PHE	N-CA-C	5.19	112.89	108.22

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	3500	0	3431	7	0
1	B	3512	0	3442	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3508	0	3438	5	0
1	D	3500	0	3425	5	0
2	E	16	0	20	0	0
2	F	16	0	20	0	0
2	G	16	0	20	0	0
2	H	16	0	20	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	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	270	0	0	0	0
6	B	344	0	0	0	0
6	C	137	0	0	0	0
6	D	337	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	H	2	0	0	0	0
All	All	15192	0	13816	20	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 1.

All (20) 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:A:33:VAL:CG1	1:B:33:VAL:CG1	2.79	0.60
1:A:33:VAL:HG11	1:B:33:VAL:CG1	2.33	0.58
1:A:206:MET:HE1	1:A:211:LEU:HD21	1.88	0.56
1:A:33:VAL:CG1	1:B:33:VAL:HG11	2.36	0.55
1:B:206:MET:HE1	1:B:211:LEU:HD21	1.92	0.51
1:C:407:ASP:OD2	1:C:425:LYS:NZ	2.39	0.50
1:D:191:THR:HG22	1:D:272:ILE:HD12	1.93	0.50
1:A:191:THR:HG22	1:A:272:ILE:HD12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ILE:HG23	1:C:7:GLU:HG2	1.97	0.47
1:D:281:LYS:NZ	1:D:431:GLU:OE2	2.49	0.46
1:D:398:TYR:HA	1:D:401:ILE:HD12	1.99	0.44
1:D:206:MET:HE1	1:D:211:LEU:HD21	2.00	0.44
1:C:60:ALA:HA	1:C:77:PHE:O	2.17	0.44
1:C:191:THR:HG22	1:C:272:ILE:HD12	1.98	0.44
1:B:3:ILE:HG23	1:B:7:GLU:HG2	1.99	0.44
1:B:398:TYR:HA	1:B:401:ILE:HD12	2.00	0.44
1:D:215:ILE:HD11	1:D:259:ILE:HG21	2.01	0.42
1:A:128:TYR:HA	1:A:163:ILE:O	2.20	0.42
1:C:128:TYR:HA	1:C:163:ILE:O	2.20	0.41
1:A:382:VAL:O	1:A:406:GLU:HA	2.21	0.41

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	438/440 (100%)	425 (97%)	13 (3%)	0	100	100
1	B	440/440 (100%)	429 (98%)	11 (2%)	0	100	100
1	C	439/440 (100%)	428 (98%)	11 (2%)	0	100	100
1	D	438/440 (100%)	427 (98%)	11 (2%)	0	100	100
All	All	1755/1760 (100%)	1709 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	370/370 (100%)	369 (100%)	1 (0%)	86	91
1	B	372/370 (100%)	371 (100%)	1 (0%)	86	91
1	C	371/370 (100%)	368 (99%)	3 (1%)	73	80
1	D	370/370 (100%)	370 (100%)	0	100	100
2	E	2/3 (67%)	2 (100%)	0	100	100
2	F	2/3 (67%)	2 (100%)	0	100	100
2	G	2/3 (67%)	2 (100%)	0	100	100
2	H	2/3 (67%)	2 (100%)	0	100	100
All	All	1491/1492 (100%)	1486 (100%)	5 (0%)	86	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	B	428	GLU
1	C	2	GLU
1	C	396	GLU
1	C	428	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	243	HIS
1	B	114	ASN
1	B	115	GLN
1	B	220	ASN
1	C	6	GLN
1	C	342	ASN
1	D	342	ASN
1	D	344	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OCS	C	249	1	6,8,9	5.61	1 (16%)	7,11,13	3.18	3 (42%)
1	OCS	A	249	1	6,8,9	5.52	2 (33%)	7,11,13	3.17	3 (42%)
1	OCS	B	249	1	6,8,9	5.47	1 (16%)	7,11,13	2.84	3 (42%)
1	OCS	D	249	1	6,8,9	5.39	1 (16%)	7,11,13	2.39	3 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	C	249	1	-	0/4/7/9	-
1	OCS	A	249	1	-	0/4/7/9	-
1	OCS	B	249	1	-	0/4/7/9	-
1	OCS	D	249	1	-	0/4/7/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	249	OCS	OD1-SG	13.54	1.83	1.45
1	A	249	OCS	OD1-SG	13.28	1.82	1.45
1	B	249	OCS	OD1-SG	13.23	1.82	1.45
1	D	249	OCS	OD1-SG	12.88	1.81	1.45
1	A	249	OCS	OD3-SG	2.01	1.50	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	OCS	OD3-SG-CB	7.13	117.41	106.76
1	C	249	OCS	OD3-SG-CB	5.53	115.02	106.76
1	B	249	OCS	OD3-SG-CB	5.39	114.80	106.76
1	D	249	OCS	OD1-SG-CB	-4.97	99.33	106.76
1	C	249	OCS	OD1-SG-CB	-4.81	99.57	106.76
1	B	249	OCS	OD1-SG-CB	-4.73	99.69	106.76
1	A	249	OCS	OD1-SG-CB	-3.50	101.53	106.76
1	C	249	OCS	OD2-SG-CB	3.44	112.61	105.97
1	D	249	OCS	OD2-SG-CB	2.59	110.97	105.97
1	D	249	OCS	OD3-SG-CB	2.58	110.61	106.76
1	B	249	OCS	CA-CB-SG	-2.17	110.38	113.61
1	A	249	OCS	OD2-SG-CB	-2.08	101.95	105.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 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

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	439/440 (99%)	0.73	34 (7%)	19 18	27, 36, 60, 85	1 (0%)
1	B	438/440 (99%)	0.29	21 (4%)	35 34	23, 36, 60, 85	5 (1%)
1	C	438/440 (99%)	1.32	119 (27%)	1 1	22, 36, 60, 85	4 (0%)
1	D	438/440 (99%)	0.46	34 (7%)	19 18	28, 36, 59, 85	2 (0%)
2	E	2/3 (66%)	3.60	2 (100%)	0 0	40, 40, 40, 42	2 (100%)
2	F	2/3 (66%)	4.66	2 (100%)	0 0	36, 36, 36, 38	2 (100%)
2	G	2/3 (66%)	6.98	2 (100%)	0 0	47, 47, 47, 47	2 (100%)
2	H	2/3 (66%)	4.41	2 (100%)	0 0	39, 39, 39, 40	2 (100%)
All	All	1761/1772 (99%)	0.72	216 (12%)	8 7	22, 36, 60, 85	20 (1%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	2	LEU	8.0
1	A	440	GLN	7.7
1	C	358	LEU	7.6
1	A	89	PHE	7.1
2	F	2	LEU	5.9
2	G	1	PRO	5.9
1	A	83	LEU	5.9
1	C	363	VAL	5.9
1	D	83	LEU	5.8
1	C	89	PHE	5.5
1	D	89	PHE	5.5
1	D	70	THR	5.4
1	C	173	ARG	5.3
1	C	268	TYR	5.1
1	C	88	TRP	5.1
1	C	357	GLY	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	226	TYR	5.1
1	B	89	PHE	4.9
1	C	181	ILE	4.9
2	H	2	LEU	4.8
1	D	243	HIS	4.5
1	C	179	GLU	4.5
1	D	84	THR	4.5
1	C	364	GLY	4.5
1	C	178	PRO	4.5
1	C	174	LEU	4.5
1	A	87	ILE	4.5
1	C	185[A]	ARG	4.5
1	C	439	LYS	4.5
1	B	83	LEU	4.4
1	C	365	VAL	4.3
1	D	85	ALA	4.3
1	C	177	SER	4.2
1	D	88	TRP	4.2
1	B	243	HIS	4.1
1	A	88	TRP	4.1
2	E	2	LEU	4.1
2	H	1	PRO	4.1
1	C	225	ARG	4.0
1	C	175	PHE	4.0
1	C	183	VAL	4.0
1	C	190	ILE	4.0
1	C	284	GLN	3.9
1	C	241	ILE	3.7
1	C	359	ASP	3.7
1	C	355	TRP	3.6
1	B	38	ASP	3.6
1	C	410	VAL	3.6
1	D	38	ASP	3.5
1	C	1	SER	3.5
1	C	330	ILE	3.5
1	C	83	LEU	3.5
1	C	390	PRO	3.4
2	F	1	PRO	3.4
1	C	90	GLY	3.4
1	B	88	TRP	3.3
1	C	243	HIS	3.3
1	C	394	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	84	THR	3.2
1	C	366	TYR	3.2
1	C	360	VAL	3.2
1	C	396	GLU	3.2
1	C	325	LEU	3.2
1	C	417	GLU	3.2
1	B	349	MET	3.2
2	E	1	PRO	3.1
1	A	84	THR	3.1
1	A	38	ASP	3.1
1	C	228	SER	3.1
1	C	254	GLY	3.1
1	B	17	GLU	3.1
1	D	86	GLU	3.0
1	C	184	LEU	3.0
1	C	362	ASP	3.0
1	C	430	ILE	3.0
1	B	155	ASN	3.0
1	A	396	GLU	3.0
1	B	70	THR	3.0
1	C	265	TYR	3.0
1	C	224	ALA	2.9
1	C	331	LEU	2.9
1	D	87	ILE	2.9
1	A	85	ALA	2.9
1	B	82	ASP	2.9
1	C	87	ILE	2.9
1	A	154	GLN	2.9
1	C	176	LYS	2.9
1	C	327	LYS	2.9
1	C	392	ALA	2.9
1	C	186	ARG	2.9
1	C	227	PRO	2.9
1	C	282	PHE	2.9
1	D	439	LYS	2.9
1	C	223	GLY	2.8
1	C	236	GLY	2.8
1	B	1	SER	2.8
1	C	333	GLY	2.8
1	C	340	ALA	2.8
1	A	86	GLU	2.7
1	C	291	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	367	GLY	2.7
1	C	370	ARG	2.7
1	C	286	GLN	2.7
1	C	373	ILE	2.7
1	C	180	GLU	2.7
1	D	82	ASP	2.7
1	A	90	GLY	2.7
1	C	377	GLY	2.7
1	B	439	LYS	2.7
1	C	305	ARG	2.7
1	D	414	THR	2.7
1	D	155	ASN	2.7
1	B	90	GLY	2.7
1	B	85	ALA	2.7
1	C	389	ALA	2.7
1	A	217	HIS	2.7
1	C	349	MET	2.7
1	C	380	LEU	2.6
1	C	414	THR	2.6
1	C	413	GLU	2.6
1	C	283	THR	2.6
1	C	411	ILE	2.6
1	D	71	HIS	2.6
1	C	345	ARG	2.6
1	C	371	SER	2.6
1	B	84	THR	2.6
1	D	153	ARG	2.6
1	C	342	ASN	2.5
1	C	308	THR	2.5
1	D	40	GLU	2.5
1	C	82	ASP	2.5
1	C	264	GLU	2.5
1	C	419	LEU	2.5
1	D	242	LEU	2.5
1	A	215	ILE	2.5
1	A	209	TYR	2.5
1	C	97	ALA	2.5
1	A	252	ARG	2.5
1	C	221	ARG	2.5
1	A	146	GLU	2.4
1	C	182	ALA	2.4
1	C	329	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	87	ILE	2.4
1	C	393	GLU	2.4
1	A	226	TYR	2.4
1	D	41	TYR	2.4
1	A	221	ARG	2.4
1	C	415	GLY	2.4
1	A	240	CYS	2.4
1	A	345	ARG	2.4
1	B	240	CYS	2.4
1	D	81	ARG	2.4
1	C	277	PRO	2.4
1	C	361	HIS	2.4
1	C	240	CYS	2.4
1	A	246	GLU	2.3
1	A	155	ASN	2.3
1	A	82	ASP	2.3
1	A	332	LYS	2.3
1	A	207	PHE	2.3
1	C	222	HIS	2.3
1	C	220	ASN	2.3
1	C	269	ALA	2.3
1	C	307	GLY	2.3
1	C	328	LEU	2.3
1	C	347	PHE	2.2
1	C	335	VAL	2.2
1	B	345	ARG	2.2
1	C	252	ARG	2.2
1	C	263	CYS	2.2
1	C	428	GLU	2.2
1	B	71	HIS	2.2
1	C	368	GLN	2.2
1	C	323	SER	2.2
1	D	1	SER	2.2
1	A	153	ARG	2.2
1	C	326	VAL	2.2
1	D	42	PRO	2.2
1	D	80	VAL	2.2
1	B	86	GLU	2.2
1	C	437	ALA	2.2
1	C	91	ARG	2.2
1	C	356	LEU	2.2
1	A	79[A]	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	220	ASN	2.2
1	B	96	ASP	2.2
1	D	43	TYR	2.1
1	A	334	ASP	2.1
1	C	388	ILE	2.1
1	A	243	HIS	2.1
1	D	33	VAL	2.1
1	C	372	ARG	2.1
1	D	252	ARG	2.1
1	C	374	LEU	2.1
1	D	67	SER	2.1
1	C	378	MET	2.1
1	D	17	GLU	2.1
1	A	96	ASP	2.1
1	C	69	ASP	2.1
1	D	90	GLY	2.1
1	C	85	ALA	2.1
1	C	230	ASN	2.1
1	C	38	ASP	2.1
1	C	391	ASP	2.1
1	C	376	PRO	2.1
1	D	241	ILE	2.1
1	C	187	ALA	2.1
1	D	112	GLU	2.0
1	D	96	ASP	2.0
1	A	225	ARG	2.0
1	C	70	THR	2.0
1	D	68	ASP	2.0
1	D	91	ARG	2.0
1	A	70	THR	2.0
1	C	400	GLY	2.0
1	C	398	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	C	249	9/10	0.93	0.10	31,34,53,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OCS	A	249	9/10	0.94	0.12	31,34,54,56	0
1	OCS	D	249	9/10	0.95	0.11	31,34,54,58	0
1	OCS	B	249	9/10	0.97	0.09	31,34,53,59	0

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
5	CL	C	1442	1/1	0.95	0.18	53,53,53,53	0
4	MG	C	1441	1/1	0.96	0.13	49,49,49,49	0
5	CL	A	1442	1/1	0.98	0.14	47,47,47,47	0
5	CL	B	1443	1/1	0.98	0.15	39,39,39,39	0
4	MG	A	1441	1/1	0.98	0.14	32,32,32,32	0
4	MG	B	1441	1/1	0.99	0.13	27,27,27,27	0
4	MG	B	1442	1/1	0.99	0.09	44,44,44,44	0
3	ZN	B	1440	1/1	0.99	0.04	43,43,43,43	0
4	MG	D	1441	1/1	0.99	0.14	26,26,26,26	0
4	MG	D	1442	1/1	0.99	0.07	43,43,43,43	0
3	ZN	C	1440	1/1	0.99	0.05	67,67,67,67	0
3	ZN	D	1440	1/1	0.99	0.05	48,48,48,48	0
3	ZN	A	1440	1/1	0.99	0.03	50,50,50,50	0
5	CL	D	1443	1/1	0.99	0.12	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.