



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:34 AM UTC

PDB ID : 4EG2 / pdb_00004eg2
Title : 2.2 Angstrom Crystal Structure of Cytidine deaminase from *Vibrio cholerae* in Complex with Zinc and Uridine
Authors : Minasov, G.; Wawrzak, Z.; Skarina, T.; Wang, Y.; Grimshaw, S.; Papazisi, L.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2012-03-30
Resolution : 2.20 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

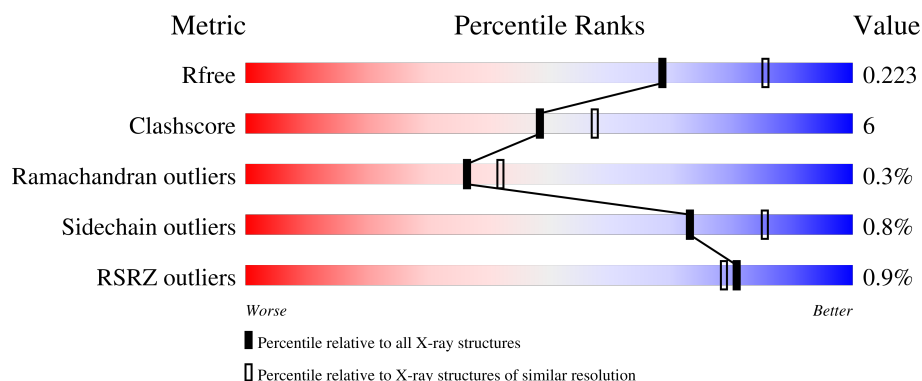
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	298	85% 14% .
1	B	298	% 94% 6%
1	C	298	% 90% 9% .
1	D	298	2% 88% 11% .

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Mol	Chain	Length	Quality of chain
1	E	298	87% 11% .
1	F	298	% 88% 10% ..
1	G	298	2% 86% 13%
1	H	298	% 86% 13% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19771 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 Cytidine deaminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	Se	0	7	0
			2317	1462	390	451	3	11			
1	B	297	Total	C	N	O	S	Se	0	4	0
			2292	1449	384	445	3	11			
1	C	296	Total	C	N	O	S	Se	0	4	0
			2279	1437	381	447	3	11			
1	D	297	Total	C	N	O	S	Se	0	5	0
			2301	1454	385	448	3	11			
1	E	297	Total	C	N	O	S	Se	0	2	0
			2276	1436	384	442	3	11			
1	F	296	Total	C	N	O	S	Se	0	1	0
			2257	1426	377	440	3	11			
1	G	297	Total	C	N	O	S	Se	0	0	0
			2256	1425	378	439	3	11			
1	H	297	Total	C	N	O	S	Se	0	3	0
			2285	1441	384	446	3	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9KSM5
A	-1	ASN	-	expression tag	UNP Q9KSM5
A	0	ALA	-	expression tag	UNP Q9KSM5
B	-2	SER	-	expression tag	UNP Q9KSM5
B	-1	ASN	-	expression tag	UNP Q9KSM5
B	0	ALA	-	expression tag	UNP Q9KSM5
C	-2	SER	-	expression tag	UNP Q9KSM5
C	-1	ASN	-	expression tag	UNP Q9KSM5
C	0	ALA	-	expression tag	UNP Q9KSM5
D	-2	SER	-	expression tag	UNP Q9KSM5
D	-1	ASN	-	expression tag	UNP Q9KSM5
D	0	ALA	-	expression tag	UNP Q9KSM5
E	-2	SER	-	expression tag	UNP Q9KSM5

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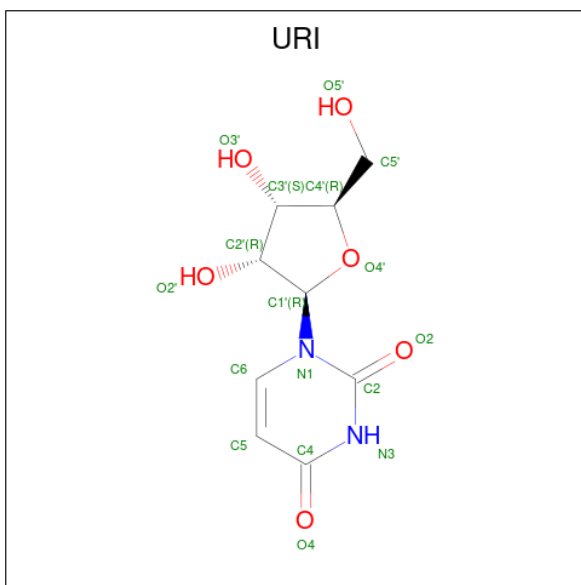
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q9KSM5
E	0	ALA	-	expression tag	UNP Q9KSM5
F	-2	SER	-	expression tag	UNP Q9KSM5
F	-1	ASN	-	expression tag	UNP Q9KSM5
F	0	ALA	-	expression tag	UNP Q9KSM5
G	-2	SER	-	expression tag	UNP Q9KSM5
G	-1	ASN	-	expression tag	UNP Q9KSM5
G	0	ALA	-	expression tag	UNP Q9KSM5
H	-2	SER	-	expression tag	UNP Q9KSM5
H	-1	ASN	-	expression tag	UNP Q9KSM5
H	0	ALA	-	expression tag	UNP Q9KSM5

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

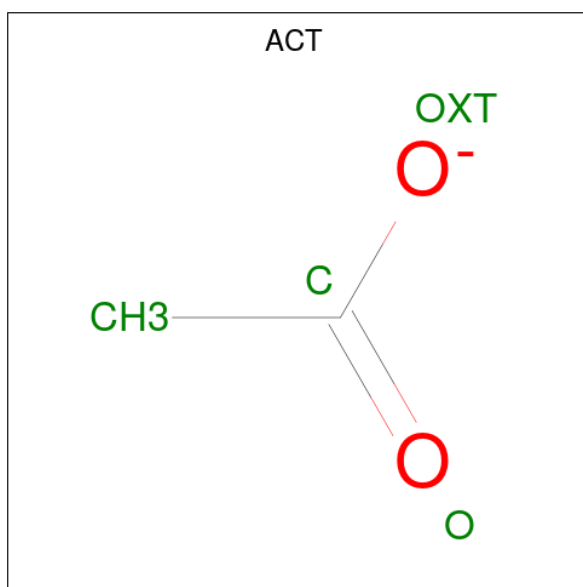
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

- Molecule 3 is URIDINE (CCD ID: URI) (formula: C₉H₁₂N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	2	6		
3	B	1	Total	C	N	O	0	0
			17	9	2	6		
3	C	1	Total	C	N	O	0	0
			17	9	2	6		
3	D	1	Total	C	N	O	0	0
			17	9	2	6		
3	E	1	Total	C	N	O	0	0
			17	9	2	6		
3	F	1	Total	C	N	O	0	0
			17	9	2	6		
3	G	1	Total	C	N	O	0	0
			17	9	2	6		
3	H	1	Total	C	N	O	0	0
			17	9	2	6		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

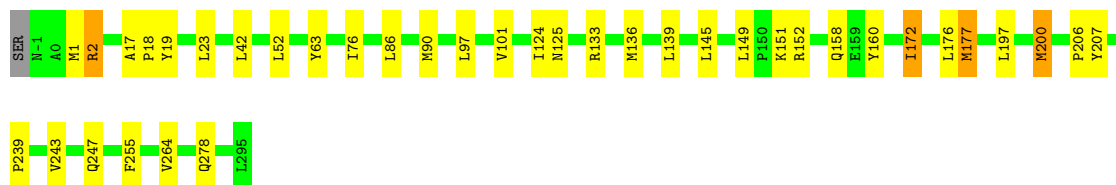
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	183	Total 185	O 185	0	4
6	B	223	Total 224	O 224	0	1
6	C	177	Total 178	O 178	0	1
6	D	182	Total 182	O 182	0	0
6	E	156	Total 157	O 157	0	1
6	F	163	Total 167	O 167	0	4
6	G	111	Total 111	O 111	0	0
6	H	122	Total 123	O 123	0	1

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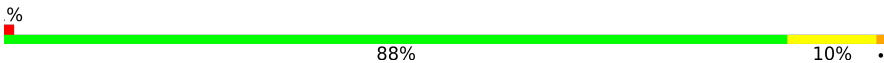
- Molecule 1: Cytidine deaminase

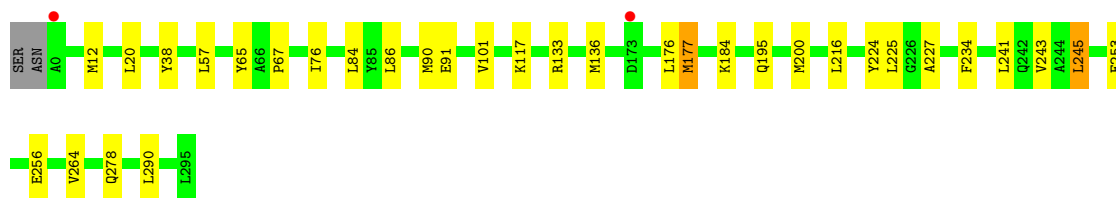


Chain E:  87% 11% .



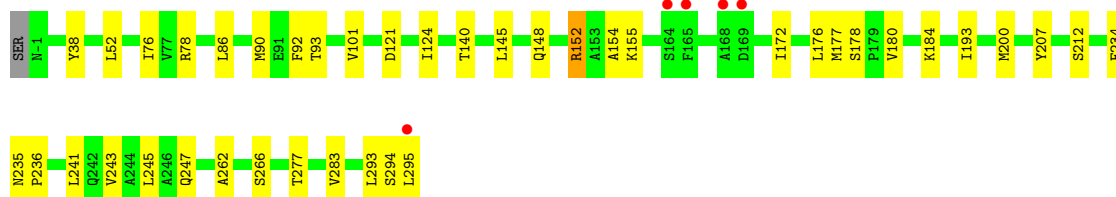
• Molecule 1: Cytidine deaminase

Chain F:  88% 10% ..



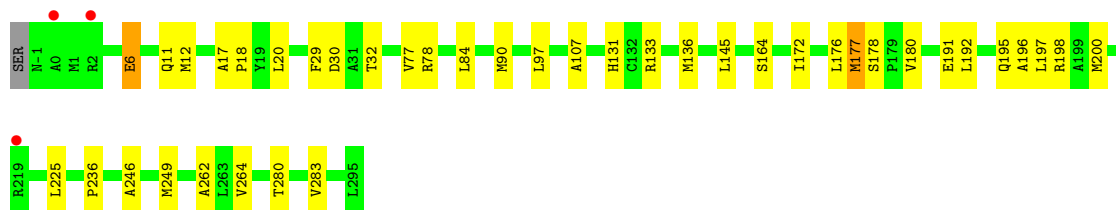
• Molecule 1: Cytidine deaminase

Chain G:  86% 13%



• Molecule 1: Cytidine deaminase

Chain H:  86% 13% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.81Å 163.73Å 111.95Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	40.21 – 2.20 40.21 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.21-2.20) 98.9 (40.21-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.159 , 0.210 0.173 , 0.223	Depositor DCC
R_{free} test set	6173 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19771	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.40% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.71	0/2351	0.89	2/3170 (0.1%)
1	B	0.68	0/2326	0.85	1/3137 (0.0%)
1	C	0.68	0/2312	0.88	3/3118 (0.1%)
1	D	0.66	0/2335	0.85	0/3149
1	E	0.64	0/2309	0.87	3/3113 (0.1%)
1	F	0.67	0/2290	0.86	0/3088
1	G	0.58	0/2289	0.83	0/3087
1	H	0.61	0/2318	0.89	3/3125 (0.1%)
All	All	0.66	0/18530	0.87	12/24987 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	172	ILE	N-CA-C	5.84	117.25	108.96
1	H	29	PHE	N-CA-C	5.68	119.05	110.64
1	A	211	PHE	N-CA-C	-5.56	102.16	110.23
1	H	164	SER	N-CA-C	5.33	117.56	110.53
1	A	165	PHE	N-CA-C	-5.32	101.03	109.96
1	E	172	ILE	N-CA-C	5.32	115.61	108.17
1	E	239	PRO	N-CA-C	5.30	115.56	110.47
1	E	139	LEU	N-CA-C	5.11	117.70	110.50
1	B	165	PHE	N-CA-C	-5.09	101.42	109.76
1	C	165	PHE	N-CA-C	-5.07	101.45	109.76
1	C	166	GLY	CA-C-N	5.01	124.46	119.24
1	C	166	GLY	C-N-CA	5.01	124.46	119.24

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	2317	0	2276	27	0
1	B	2292	0	2257	13	0
1	C	2279	0	2238	19	0
1	D	2301	0	2262	25	0
1	E	2276	0	2244	30	0
1	F	2257	0	2224	23	0
1	G	2256	0	2225	35	0
1	H	2285	0	2247	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	17	0	12	0	0
3	B	17	0	12	0	0
3	C	17	0	12	0	0
3	D	17	0	12	0	0
3	E	17	0	12	0	0
3	F	17	0	12	0	0
3	G	17	0	12	0	0
3	H	17	0	12	0	0
4	A	4	0	3	0	0
4	B	4	0	3	1	0
4	D	8	0	6	0	0
4	E	12	0	9	1	0
4	F	4	0	3	1	0
4	G	4	0	3	0	0
5	B	1	0	0	0	0
6	A	185	0	0	5	0
6	B	224	0	0	2	0
6	C	178	0	0	3	0
6	D	182	0	0	5	0
6	E	157	0	0	1	0
6	F	167	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	111	0	0	2	0
6	H	123	0	0	1	0
All	All	19771	0	18096	202	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 6.

All (202) 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:H:200:MSE:CE	1:H:264:VAL:HG12	1.62	1.29
1:H:200:MSE:HE3	1:H:264:VAL:HG12	1.18	1.10
1:H:200:MSE:HE3	1:H:264:VAL:CG1	1.87	1.04
1:B:125[A]:ASN:HD22	1:B:125[A]:ASN:N	1.54	0.99
1:B:125[A]:ASN:ND2	1:B:125[A]:ASN:H	1.49	0.97
1:G:93:THR:O	1:G:283:VAL:HG11	1.66	0.95
1:E:172:ILE:HD13	1:E:206:PRO:HB2	1.53	0.89
1:E:172:ILE:HD12	1:E:207:TYR:CE1	2.10	0.86
1:F:216:LEU:HD11	1:F:245:LEU:HD13	1.59	0.84
1:E:90:MSE:HE2	1:E:101:VAL:HG21	1.58	0.84
1:G:93:THR:O	1:G:283:VAL:CG1	2.26	0.82
1:B:125[A]:ASN:HD22	1:B:125[A]:ASN:H	0.80	0.78
1:G:200:MSE:HG3	1:G:212:SER:HA	1.64	0.78
1:E:90:MSE:CE	1:E:101:VAL:HG21	2.14	0.77
1:E:90:MSE:HE2	1:E:101:VAL:CG2	2.14	0.77
1:H:90:MSE:HE2	1:H:249:MSE:CE	2.17	0.75
1:H:90:MSE:HE1	1:H:246:ALA:HA	1.73	0.71
1:G:184:LYS:HG3	1:G:200:MSE:HE1	1.73	0.70
1:G:152:ARG:HG2	1:G:152:ARG:HH11	1.57	0.70
1:G:293:LEU:C	1:G:293:LEU:HD23	2.18	0.69
1:G:152:ARG:HH11	1:G:152:ARG:CG	2.07	0.67
1:H:90:MSE:HE2	1:H:249:MSE:HE2	1.77	0.66
1:E:1:MSE:HE3	1:E:63:TYR:CZ	2.31	0.66
1:D:124[A]:ILE:HD11	1:D:128:PRO:HD3	1.79	0.63
1:G:293:LEU:HD23	1:G:294:SER:N	2.14	0.63
1:B:7:GLN:HG2	6:B:448:HOH:O	1.99	0.63
1:C:184:LYS:HG3	1:C:200:MSE:HE1	1.81	0.63
1:G:145:LEU:C	1:G:145:LEU:HD12	2.23	0.63
1:C:214:VAL:HG23	1:C:240:PRO:HB2	1.80	0.62
1:D:200:MSE:HE2	1:D:200:MSE:C	2.25	0.62
1:F:133:ARG:HA	1:F:136:MSE:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:MSE:HG3	1:C:212:SER:HA	1.81	0.61
1:H:200:MSE:HE1	1:H:264:VAL:HG12	1.73	0.61
1:D:90:MSE:HE1	1:D:246:ALA:HA	1.82	0.61
1:F:76:ILE:HG12	1:F:86:LEU:HD22	1.81	0.61
1:E:172:ILE:HD13	1:E:206:PRO:CB	2.28	0.60
1:A:152:ARG:HG3	6:A:443:HOH:O	2.01	0.59
1:H:200:MSE:CE	1:H:264:VAL:CG1	2.54	0.59
1:C:90:MSE:HE2	1:C:249:MSE:CE	2.33	0.58
1:F:256:GLU:HG3	6:F:486:HOH:O	2.03	0.58
1:D:90:MSE:HE2	1:D:249:MSE:CE	2.33	0.58
1:F:38:TYR:CD1	1:F:84:LEU:HD11	2.39	0.58
1:F:184:LYS:HG3	1:F:200:MSE:HE2	1.86	0.58
1:D:131:HIS:CE1	1:D:236:PRO:HA	2.40	0.56
1:A:131:HIS:CE1	1:A:236:PRO:HA	2.40	0.56
1:B:255:PHE:CE2	4:B:304:ACT:H3	2.40	0.56
1:D:90:MSE:HE2	1:D:249:MSE:SE	2.55	0.56
1:A:78:ARG:HA	1:A:84:LEU:HD23	1.86	0.56
1:D:217:LYS:HE2	6:D:477:HOH:O	2.05	0.56
1:G:78:ARG:HB3	1:G:121:ASP:OD1	2.06	0.56
1:G:193:ILE:HD13	1:G:262:ALA:HB1	1.88	0.56
1:F:216:LEU:CD1	1:F:245:LEU:HD13	2.34	0.56
1:A:186:SER:HB2	1:A:295:LEU:HD11	1.88	0.55
1:H:195:GLN:O	1:H:198:ARG:HB2	2.07	0.54
1:H:280:THR:O	1:H:283:VAL:HG22	2.07	0.54
1:C:184:LYS:CG	1:C:200:MSE:HE1	2.36	0.54
1:E:76:ILE:HG12	1:E:86:LEU:HD22	1.89	0.54
1:G:155:LYS:NZ	6:G:435:HOH:O	2.39	0.54
1:G:184:LYS:CG	1:G:200:MSE:HE1	2.38	0.54
1:G:172:ILE:HD12	1:G:207:TYR:CE1	2.43	0.53
1:E:145:LEU:HD12	1:E:145:LEU:C	2.32	0.53
1:A:270:LYS:NZ	6:A:524:HOH:O	2.42	0.53
1:C:195:GLN:HB3	1:C:225:LEU:HD21	1.91	0.53
1:G:38:TYR:CE1	1:G:52:LEU:HD23	2.43	0.53
1:H:195:GLN:HB3	1:H:225:LEU:HD21	1.90	0.53
1:H:6[A]:GLU:N	1:H:6[A]:GLU:OE2	2.42	0.53
1:A:135:PHE:HA	1:A:231:ASN:ND2	2.24	0.52
1:C:90:MSE:HE2	1:C:249:MSE:HE2	1.92	0.52
1:H:17:ALA:HB3	1:H:18:PRO:HD3	1.90	0.52
1:D:145:LEU:HD12	1:D:145:LEU:C	2.35	0.52
1:A:295:LEU:HD23	1:A:295:LEU:O	2.10	0.52
1:D:165:PHE:HA	1:D:169:ASP:OD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:MSE:HE2	1:B:101:VAL:HG21	1.92	0.51
1:H:11:GLN:NE2	6:H:513:HOH:O	2.44	0.51
1:A:218:MSE:HE2	1:A:253:GLU:HB3	1.90	0.51
1:A:150:PRO:C	1:A:152:ARG:H	2.19	0.51
1:D:125[B]:ASN:OD1	1:D:125[B]:ASN:N	2.45	0.50
1:E:200:MSE:HE3	1:E:264:VAL:HG12	1.92	0.50
1:H:30:ASP:O	1:H:32:THR:HG23	2.11	0.50
1:G:243:VAL:O	1:G:247:GLN:HG2	2.10	0.50
1:A:3[B]:ASN:HB3	6:A:581[B]:HOH:O	2.11	0.50
1:E:172:ILE:CD1	1:E:206:PRO:HB2	2.33	0.49
1:F:57:LEU:HD23	1:F:76:ILE:HG13	1.93	0.49
1:G:200:MSE:HG3	1:G:212:SER:CA	2.40	0.49
1:H:12:MSE:HG3	1:H:20:LEU:HD23	1.94	0.49
1:A:34:SER:HA	1:A:83[B]:ARG:HG3	1.94	0.49
1:G:234:PHE:CD2	1:H:97:LEU:HD22	2.47	0.49
1:F:241:LEU:HG	1:F:245:LEU:HD22	1.95	0.49
1:D:-1:ASN:OD1	1:D:2:ARG:HG2	2.13	0.49
1:F:90:MSE:HE2	1:F:101:VAL:HG21	1.94	0.48
1:A:133:ARG:HA	1:A:136:MSE:HE3	1.95	0.48
1:B:90:MSE:HE2	1:B:101:VAL:CG2	2.44	0.48
1:H:178:SER:O	1:H:180:VAL:HG23	2.14	0.48
1:E:145:LEU:HD12	1:E:145:LEU:O	2.14	0.48
1:E:97:LEU:HD22	1:F:234:PHE:CD2	2.49	0.48
1:E:124:ILE:HG22	1:E:125:ASN:N	2.29	0.48
1:E:243:VAL:O	1:E:247:GLN:HG2	2.14	0.48
1:G:266:SER:HA	1:G:295:LEU:O	2.14	0.48
1:B:172:ILE:HG22	1:B:173:ASP:O	2.14	0.47
1:C:17:ALA:HB3	1:C:18:PRO:HD3	1.95	0.47
1:E:278:GLN:HG3	6:E:513:HOH:O	2.12	0.47
1:A:172:ILE:HD13	1:A:206:PRO:HB2	1.96	0.47
1:G:90:MSE:HE2	1:G:101:VAL:HG21	1.96	0.47
1:A:129:CYS:O	1:A:133:ARG:HG3	2.15	0.47
1:D:150:PRO:O	1:D:151:LYS:HG2	2.14	0.47
1:G:90:MSE:HE3	1:G:92:PHE:CZ	2.50	0.47
1:H:145:LEU:HD12	1:H:145:LEU:C	2.40	0.47
1:G:293:LEU:C	1:G:293:LEU:CD2	2.87	0.47
1:H:133:ARG:HA	1:H:136:MSE:HE3	1.97	0.47
1:A:12:MSE:HE3	1:A:59:ILE:HD11	1.97	0.47
1:F:216:LEU:CD1	1:F:245:LEU:CD1	2.93	0.46
1:D:146:LYS:NZ	6:D:491:HOH:O	2.48	0.46
1:G:90:MSE:HE2	1:G:101:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:LEU:HD11	1:F:245:LEU:CD1	2.39	0.46
1:F:227:ALA:O	1:F:243:VAL:HG21	2.16	0.46
1:F:278:GLN:HG2	1:F:290:LEU:HD23	1.98	0.46
1:G:76:ILE:HG12	1:G:86:LEU:HD22	1.97	0.46
1:H:6[A]:GLU:OE2	1:H:6[A]:GLU:CA	2.64	0.46
1:C:145:LEU:C	1:C:145:LEU:HD12	2.41	0.46
1:E:158[B]:GLN:H	1:E:158[B]:GLN:CD	2.24	0.46
1:H:78:ARG:HA	1:H:84:LEU:HD23	1.97	0.46
1:B:125[A]:ASN:N	1:B:125[A]:ASN:ND2	2.26	0.45
1:B:17:ALA:HB3	1:B:18:PRO:HD3	1.99	0.45
1:D:10:GLN:HG2	6:D:468:HOH:O	2.15	0.45
1:D:150:PRO:C	1:D:151:LYS:HG2	2.41	0.45
1:G:90:MSE:HE3	1:G:92:PHE:HZ	1.81	0.45
1:G:152:ARG:CG	1:G:152:ARG:NH1	2.74	0.45
1:H:197:LEU:HD12	1:H:200:MSE:HG2	1.97	0.45
1:D:125[A]:ASN:ND2	6:D:473:HOH:O	2.49	0.45
1:C:129:CYS:O	1:C:133:ARG:HG3	2.17	0.45
1:D:214:VAL:HG23	1:D:240:PRO:HB2	1.98	0.45
1:G:184:LYS:CB	1:G:200:MSE:HE1	2.46	0.45
1:A:180:VAL:HG23	1:A:202:ILE:HA	1.99	0.45
1:D:129:CYS:O	1:D:133:ARG:HG3	2.16	0.45
1:A:150:PRO:O	1:A:152:ARG:N	2.49	0.45
1:B:38:TYR:CE1	1:B:52:LEU:HD23	2.52	0.44
1:D:124[A]:ILE:HD11	1:D:149:LEU:HD21	1.99	0.44
1:E:176:LEU:O	1:E:177:MSE:HB2	2.17	0.44
1:A:9:LEU:HD11	1:A:24:VAL:CG2	2.47	0.44
1:A:198:ARG:HD2	6:A:452:HOH:O	2.16	0.44
1:B:218:MSE:HE2	1:B:253:GLU:HB3	2.00	0.44
1:C:11:GLN:HB2	6:C:439:HOH:O	2.18	0.44
1:E:90:MSE:CE	1:E:101:VAL:CG2	2.87	0.44
1:H:200:MSE:HE2	1:H:264:VAL:C	2.43	0.44
1:D:167:PRO:HB2	6:D:426:HOH:O	2.18	0.44
1:C:90:MSE:HE1	1:C:246:ALA:HA	2.00	0.43
1:H:192:LEU:HG	1:H:262:ALA:CB	2.48	0.43
1:G:140:THR:HA	6:G:503:HOH:O	2.18	0.43
1:G:176:LEU:O	1:G:177:MSE:HB2	2.18	0.43
1:A:17:ALA:HB3	1:A:18:PRO:HD3	2.01	0.43
1:F:67:PRO:HD2	1:F:91:GLU:HB2	2.01	0.43
1:F:65:TYR:HB2	4:F:303:ACT:H2	2.00	0.43
1:F:200:MSE:SE	1:F:264:VAL:HG12	2.69	0.43
1:C:218:MSE:HE2	1:C:253:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:VAL:HG13	1:D:119:VAL:HG13	2.01	0.43
1:E:149:LEU:HD22	1:E:160:TYR:OH	2.19	0.43
1:C:133:ARG:HA	1:C:136:MSE:HE3	2.00	0.43
1:E:42:LEU:HA	1:E:52:LEU:HD22	2.01	0.43
1:F:176:LEU:O	1:F:177:MSE:HB2	2.19	0.43
1:D:57:LEU:N	1:D:58:PRO:CD	2.82	0.42
1:D:184:LYS:HG3	1:D:200:MSE:HE1	2.01	0.42
1:G:241:LEU:HD22	1:G:277:THR:HG23	2.00	0.42
1:A:104:GLU:CG	1:A:124[B]:ILE:HD13	2.48	0.42
1:B:256:GLU:HG2	6:B:543:HOH:O	2.18	0.42
1:E:19:TYR:CE2	1:E:23:LEU:HD11	2.54	0.42
1:E:255:PHE:H	4:E:303:ACT:H1	1.84	0.42
1:F:195:GLN:HB3	1:F:225:LEU:HD21	2.00	0.42
1:F:224:TYR:CE2	1:F:253:GLU:HG3	2.55	0.42
1:H:176:LEU:O	1:H:177:MSE:HB2	2.20	0.42
1:A:165:PHE:HA	1:A:169:ASP:OD2	2.19	0.42
1:E:197:LEU:HD12	1:E:200:MSE:HG2	2.01	0.42
1:C:78:ARG:HB2	1:C:84:LEU:CD2	2.50	0.42
1:C:90:MSE:HE3	1:C:90:MSE:HB2	1.88	0.42
1:D:178:SER:O	1:D:180:VAL:HG23	2.20	0.42
1:E:2:ARG:NE	1:E:2:ARG:HA	2.34	0.42
1:A:243:VAL:O	1:A:247:GLN:HG2	2.20	0.41
1:E:17:ALA:HB3	1:E:18:PRO:HD3	2.01	0.41
1:G:178:SER:O	1:G:180:VAL:HG23	2.20	0.41
1:H:191[A]:GLU:HA	1:H:191[A]:GLU:OE1	2.20	0.41
1:C:135:PHE:HA	1:C:231:ASN:ND2	2.36	0.41
1:G:145:LEU:HD12	1:G:145:LEU:O	2.20	0.41
1:G:235:ASN:N	1:G:236:PRO:CD	2.84	0.41
1:H:196:ALA:HB3	1:H:264:VAL:HG23	2.03	0.41
1:C:158:GLN:HG3	6:C:425:HOH:O	2.20	0.41
1:F:12:MSE:HG3	1:F:20:LEU:HD23	2.03	0.41
1:H:131:HIS:CE1	1:H:236:PRO:HA	2.56	0.41
1:A:217:LYS:HD2	6:A:504:HOH:O	2.19	0.41
1:H:77:VAL:HG23	1:H:107:ALA:HB1	2.02	0.41
1:A:145:LEU:HD12	1:A:145:LEU:C	2.46	0.41
1:C:114:LYS:HE3	6:C:442:HOH:O	2.20	0.41
1:E:1:MSE:CE	1:E:63:TYR:CZ	3.02	0.41
1:G:92:PHE:CZ	1:G:245:LEU:HD13	2.56	0.41
1:H:200:MSE:HE3	1:H:264:VAL:HG11	1.91	0.41
1:A:217:LYS:HA	1:A:223:ILE:HD13	2.01	0.40
1:H:90:MSE:HE3	1:H:90:MSE:HB2	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:ARG:HA	1:E:136:MSE:HE3	2.02	0.40
1:E:151:LYS:O	1:E:152:ARG:HG2	2.21	0.40
1:D:73:VAL:HA	1:D:125[B]:ASN:HD21	1.87	0.40
1:E:158[B]:GLN:CD	1:E:158[B]:GLN:N	2.79	0.40
1:G:148:GLN:OE1	1:G:154:ALA:HB2	2.22	0.40
1:A:176:LEU:O	1:A:177:MSE:HB2	2.21	0.40
1:F:76:ILE:HG12	1:F:86:LEU:CD2	2.51	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	302/298 (101%)	298 (99%)	2 (1%)	2 (1%)	18	19
1	B	299/298 (100%)	293 (98%)	5 (2%)	1 (0%)	36	42
1	C	298/298 (100%)	292 (98%)	6 (2%)	0	100	100
1	D	300/298 (101%)	294 (98%)	5 (2%)	1 (0%)	36	42
1	E	297/298 (100%)	293 (99%)	3 (1%)	1 (0%)	36	42
1	F	295/298 (99%)	292 (99%)	2 (1%)	1 (0%)	36	42
1	G	295/298 (99%)	290 (98%)	5 (2%)	0	100	100
1	H	298/298 (100%)	291 (98%)	6 (2%)	1 (0%)	36	42
All	All	2384/2384 (100%)	2343 (98%)	34 (1%)	7 (0%)	36	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	LYS
1	F	177	MSE
1	A	177	MSE

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Mol	Chain	Res	Type
1	D	177	MSE
1	B	177	MSE
1	H	177	MSE
1	E	177	MSE

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	244/227 (108%)	242 (99%)	2 (1%)	73	85
1	B	241/227 (106%)	236 (98%)	5 (2%)	47	63
1	C	240/227 (106%)	239 (100%)	1 (0%)	84	92
1	D	242/227 (107%)	240 (99%)	2 (1%)	73	85
1	E	239/227 (105%)	237 (99%)	2 (1%)	73	85
1	F	237/227 (104%)	235 (99%)	2 (1%)	73	85
1	G	237/227 (104%)	235 (99%)	2 (1%)	73	85
1	H	240/227 (106%)	238 (99%)	2 (1%)	73	85
All	All	1920/1816 (106%)	1902 (99%)	18 (1%)	73	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	219	ARG
1	B	11	GLN
1	B	124[A]	ILE
1	B	124[B]	ILE
1	B	125[A]	ASN
1	B	125[B]	ASN
1	C	219	ARG
1	D	184	LYS
1	D	200	MSE
1	E	2	ARG

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Mol	Chain	Res	Type
1	E	200	MSE
1	F	117	LYS
1	F	245	LEU
1	G	124	ILE
1	G	152	ARG
1	H	6[A]	GLU
1	H	6[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	39	GLN
1	B	158	GLN
1	C	11	GLN
1	C	125	ASN
1	C	209	GLN
1	C	278	GLN
1	D	39	GLN
1	E	39	GLN
1	F	11	GLN
1	F	209	GLN
1	G	137	ASN
1	G	209	GLN
1	H	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 9 are monoatomic - leaving 17 for Mogul analysis.

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
4	ACT	A	303	-	3,3,3	0.78	0	3,3,3	1.47	0
3	URI	F	302	-	18,18,18	0.35	0	26,26,26	0.58	0
3	URI	D	302	-	18,18,18	0.43	0	26,26,26	0.68	0
3	URI	G	302	-	18,18,18	0.55	0	26,26,26	0.59	0
4	ACT	G	303	-	3,3,3	0.79	0	3,3,3	1.63	1 (33%)
4	ACT	E	304	-	3,3,3	0.80	0	3,3,3	1.31	0
4	ACT	D	303	-	3,3,3	0.76	0	3,3,3	1.57	1 (33%)
3	URI	B	303	-	18,18,18	0.39	0	26,26,26	0.48	0
4	ACT	D	304	-	3,3,3	0.90	0	3,3,3	1.45	0
4	ACT	E	303	-	3,3,3	0.76	0	3,3,3	1.35	0
3	URI	H	302	2	18,18,18	0.65	0	26,26,26	0.57	0
3	URI	A	302	-	18,18,18	0.48	0	26,26,26	0.64	0
3	URI	C	302	-	18,18,18	0.49	0	26,26,26	0.70	0
3	URI	E	302	-	18,18,18	0.54	0	26,26,26	0.68	0
4	ACT	B	304	-	3,3,3	0.84	0	3,3,3	1.46	0
4	ACT	F	303	-	3,3,3	0.76	0	3,3,3	1.27	0
4	ACT	E	305	-	3,3,3	0.76	0	3,3,3	1.46	0

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
3	URI	F	302	-	-	0/6/22/22	0/2/2/2
3	URI	D	302	-	-	0/6/22/22	0/2/2/2
3	URI	G	302	-	-	0/6/22/22	0/2/2/2
3	URI	B	303	-	-	0/6/22/22	0/2/2/2
3	URI	H	302	2	-	2/6/22/22	0/2/2/2
3	URI	A	302	-	-	0/6/22/22	0/2/2/2
3	URI	C	302	-	-	0/6/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	URI	E	302	-	-	0/6/22/22	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	303	ACT	OXT-C-CH3	2.03	123.57	115.05
4	G	303	ACT	OXT-C-O	-2.01	114.56	122.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	302	URI	C3'-C4'-C5'-O5'
3	H	302	URI	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	303	ACT	1	0
4	B	304	ACT	1	0
4	F	303	ACT	1	0

5.7 Other polymers ⓘ

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	286/298 (95%)	-0.53	1 (0%) 90 88	11, 25, 44, 58	7 (2%)
1	B	286/298 (95%)	-0.60	2 (0%) 84 82	12, 26, 43, 63	4 (1%)
1	C	285/298 (95%)	-0.52	2 (0%) 84 82	18, 27, 45, 62	4 (1%)
1	D	286/298 (95%)	-0.43	6 (2%) 63 60	17, 29, 52, 75	5 (1%)
1	E	286/298 (95%)	-0.48	0 100 100	15, 32, 49, 62	2 (0%)
1	F	285/298 (95%)	-0.43	2 (0%) 84 82	17, 30, 51, 91	1 (0%)
1	G	286/298 (95%)	-0.12	5 (1%) 69 66	24, 41, 68, 110	0
1	H	286/298 (95%)	-0.26	3 (1%) 79 77	24, 37, 61, 86	3 (1%)
All	All	2286/2384 (95%)	-0.42	21 (0%) 81 79	11, 31, 55, 110	26 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	125[A]	ASN	3.7
1	C	0	ALA	3.7
1	F	173	ASP	2.8
1	F	0	ALA	2.7
1	G	165	PHE	2.5
1	G	295	LEU	2.5
1	B	126[A]	PHE	2.4
1	H	0	ALA	2.4
1	D	168	ALA	2.3
1	G	168	ALA	2.3
1	H	219[A]	ARG	2.3
1	D	0	ALA	2.3
1	H	2	ARG	2.3
1	C	126	PHE	2.3
1	D	173	ASP	2.3
1	G	169	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	126[A]	PHE	2.2
1	D	170	LEU	2.1
1	A	173	ASP	2.1
1	G	164	SER	2.0
1	B	125[A]	ASN	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
4	ACT	D	303	4/4	0.66	0.18	58,58,58,59	0
4	ACT	G	303	4/4	0.68	0.18	61,62,62,62	0
4	ACT	E	304	4/4	0.75	0.18	59,60,60,60	0
4	ACT	E	305	4/4	0.76	0.14	60,61,61,62	0
4	ACT	E	303	4/4	0.85	0.14	55,56,57,57	0
3	URI	H	302	17/17	0.85	0.14	56,62,64,65	0
4	ACT	A	303	4/4	0.86	0.12	36,37,39,39	0
4	ACT	F	303	4/4	0.87	0.17	60,61,61,61	0
4	ACT	D	304	4/4	0.88	0.13	52,53,53,53	0
4	ACT	B	304	4/4	0.89	0.11	53,53,53,54	0
3	URI	C	302	17/17	0.91	0.09	33,42,44,46	0
2	ZN	H	301	1/1	0.92	0.08	50,50,50,50	1
2	ZN	B	302	1/1	0.92	0.11	34,34,34,34	1
3	URI	E	302	17/17	0.93	0.09	31,37,40,44	0
2	ZN	F	301	1/1	0.94	0.07	40,40,40,40	1
3	URI	G	302	17/17	0.94	0.08	33,38,45,45	0
3	URI	A	302	17/17	0.94	0.07	25,31,35,36	0
2	ZN	G	301	1/1	0.94	0.07	40,40,40,40	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	D	301	1/1	0.95	0.05	32,32,32,32	1
2	ZN	A	301	1/1	0.95	0.07	36,36,36,36	1
3	URI	B	303	17/17	0.96	0.07	29,33,37,37	0
3	URI	F	302	17/17	0.97	0.05	23,30,32,33	0
2	ZN	E	301	1/1	0.97	0.04	36,36,36,36	1
3	URI	D	302	17/17	0.97	0.06	27,33,35,37	0
2	ZN	C	301	1/1	0.97	0.07	32,32,32,32	1
5	MG	B	301	1/1	0.99	0.02	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.