



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:11 AM UTC

PDB ID : 2H5E / pdb_00002h5e
Title : Crystal structure of E.coli polypeptide release factor RF3
Authors : Song, H.W.; Zhou, Z.H.
Deposited on : 2006-05-26
Resolution : 2.80 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

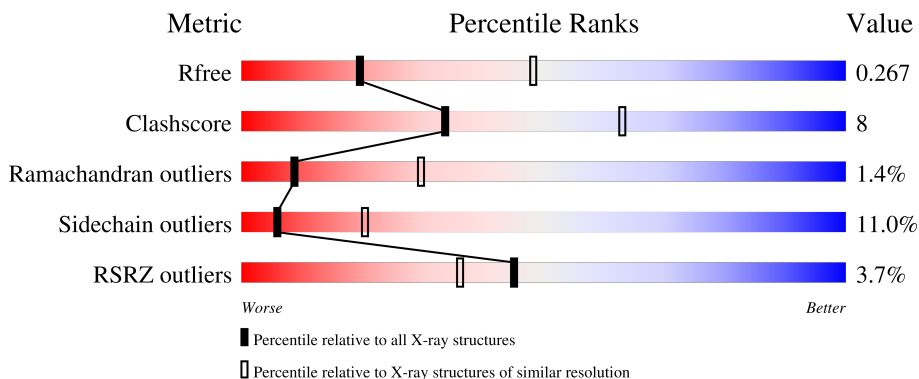
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	529	3% 69% 19% • 8%
1	B	529	4% 71% 17% • 9%

2 Entry composition [i](#)

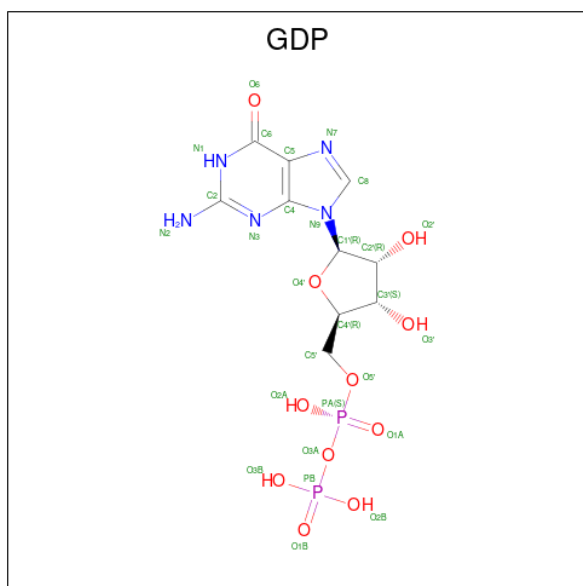
There are 3 unique types of molecules in this entry. The entry contains 7810 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peptide chain release factor RF-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3870	2454	664	732	20			
1	B	479	Total	C	N	O	S	0	0	0
			3793	2407	648	719	19			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

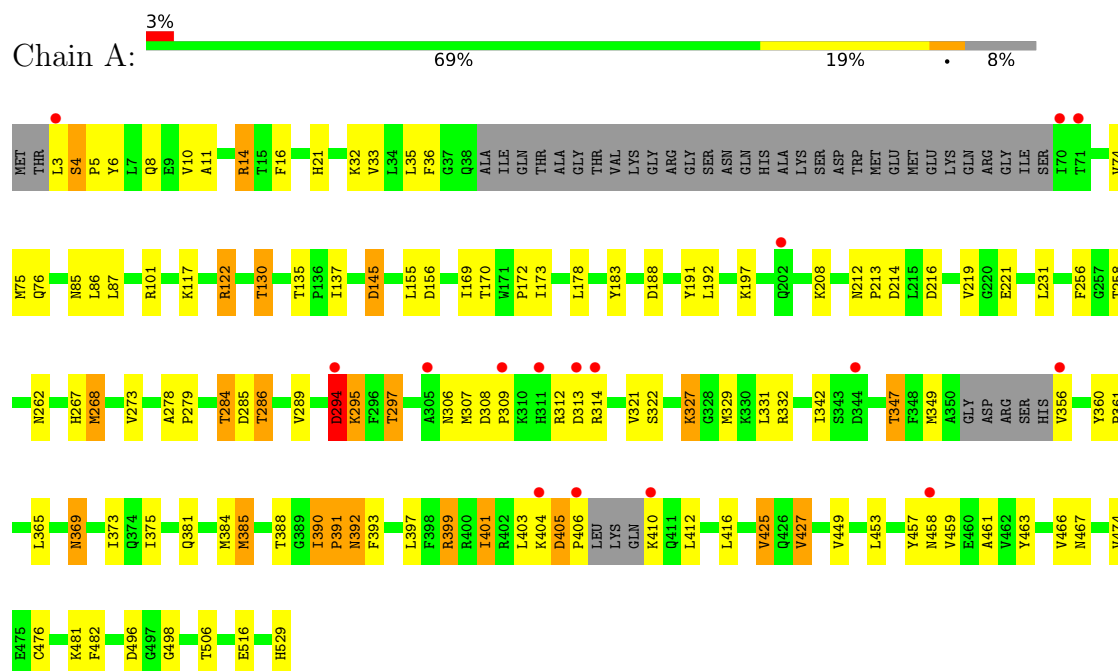
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	34	Total 34	O 34	0	0

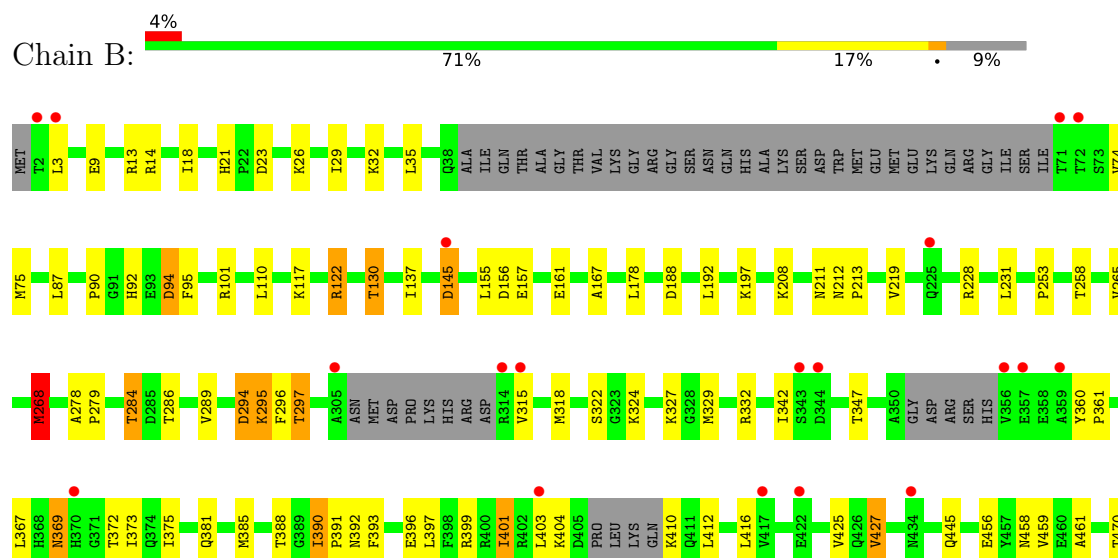
3 Residue-property plots [i](#)

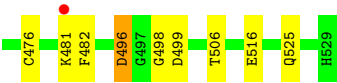
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Peptide chain release factor RF-3



• Molecule 1: Peptide chain release factor RF-3





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.17Å 239.78Å 69.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 99.1 (20.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.55 (at 2.81Å)	Xtriage
Refinement program	CNS, REFMAC 5.0	Depositor
R, R_{free}	0.225 , 0.262 0.235 , 0.267	Depositor DCC
R_{free} test set	1563 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7810	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: GDP

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	0.63	3/3941 (0.1%)	0.88	3/5324 (0.1%)
1	B	0.61	1/3860 (0.0%)	0.85	1/5213 (0.0%)
All	All	0.62	4/7801 (0.1%)	0.87	4/10537 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	268	MET	SD-CE	-7.93	1.59	1.79
1	A	268	MET	SD-CE	-5.35	1.66	1.79
1	A	385	MET	SD-CE	-5.06	1.67	1.79
1	A	384	MET	SD-CE	-5.03	1.67	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ASP	CB-CA-C	-5.67	101.38	110.79
1	A	327	LYS	N-CA-C	5.61	117.84	111.11
1	B	145	ASP	CB-CA-C	-5.43	101.45	110.68
1	A	459	VAL	N-CA-C	5.19	116.27	109.58

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	3870	0	3855	71	0
1	B	3793	0	3780	47	0
2	A	28	0	12	1	0
2	B	28	0	12	1	0
3	A	57	0	0	0	0
3	B	34	0	0	0	0
All	All	7810	0	7659	118	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 8.

All (118) 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:76:GLN:HE21	1:A:85:ASN:HD21	1.17	0.93
1:B:284:THR:HG22	1:B:286:THR:H	1.54	0.73
1:A:130:THR:HG21	1:A:137:ILE:HD11	1.71	0.70
1:B:329:MET:HE2	1:B:381:GLN:NE2	2.08	0.68
1:A:405:ASP:HB2	1:A:406:PRO:HA	1.76	0.68
1:A:405:ASP:HB2	1:A:406:PRO:CA	2.26	0.65
1:A:294:ASP:O	1:A:295:LYS:O	2.17	0.63
1:A:369:ASN:ND2	1:A:373:ILE:H	1.97	0.62
1:B:188:ASP:O	1:B:208:LYS:O	2.18	0.62
1:B:401:ILE:HG21	1:B:416:LEU:HD11	1.82	0.61
1:A:76:GLN:HE21	1:A:85:ASN:ND2	1.94	0.61
1:A:284:THR:HG22	1:A:286:THR:H	1.65	0.61
1:A:76:GLN:NE2	1:A:85:ASN:HD21	1.94	0.61
1:A:401:ILE:HD12	1:A:461:ALA:HB1	1.82	0.61
1:A:294:ASP:O	1:A:295:LYS:C	2.44	0.61
1:A:405:ASP:HB2	1:A:406:PRO:C	2.26	0.60
1:A:36:PHE:HE1	1:A:262:ASN:HD21	1.49	0.59
1:B:297:THR:HB	1:B:322:SER:OG	2.03	0.59
1:B:388:THR:O	1:B:388:THR:HG23	2.03	0.59
1:A:388:THR:HG23	1:A:388:THR:O	2.03	0.58
1:A:212:ASN:HD22	1:A:213:PRO:HD2	1.68	0.58
1:B:401:ILE:CG2	1:B:412:LEU:HD21	2.33	0.58
1:A:135:THR:O	1:A:137:ILE:HD12	2.03	0.58
1:A:212:ASN:HD22	1:A:213:PRO:CD	2.16	0.58
1:A:188:ASP:O	1:A:208:LYS:O	2.24	0.56
1:A:405:ASP:CB	1:A:406:PRO:HA	2.35	0.56
1:B:327:LYS:O	1:B:342:ILE:O	2.24	0.56
1:B:329:MET:HE2	1:B:381:GLN:HE22	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:THR:CG2	1:A:349:MET:HG2	2.36	0.55
1:A:401:ILE:CG2	1:A:412:LEU:HD21	2.36	0.54
1:A:401:ILE:HG21	1:A:416:LEU:HD11	1.89	0.54
1:A:4:SER:O	1:A:6:TYR:N	2.41	0.53
1:A:307:MET:HB2	1:A:312:ARG:HA	1.91	0.53
1:A:284:THR:CG2	1:A:385:MET:HB2	2.39	0.53
1:A:173:ILE:HG21	1:A:219:VAL:HG11	1.90	0.53
1:A:212:ASN:HD22	1:A:213:PRO:N	2.07	0.53
1:A:392:ASN:ND2	1:A:529:HIS:ND1	2.56	0.53
1:B:324:LYS:O	1:B:329:MET:HE1	2.09	0.52
1:A:401:ILE:HG23	1:A:412:LEU:HD21	1.91	0.52
1:A:295:LYS:HA	1:A:381:GLN:OE1	2.10	0.52
1:A:401:ILE:CD1	1:A:461:ALA:HB1	2.40	0.51
1:B:375:ILE:CG2	1:B:390:ILE:HD11	2.40	0.51
1:A:297:THR:HG22	1:A:321:VAL:HB	1.92	0.51
1:A:391:PRO:HG2	1:A:393:PHE:CE1	2.46	0.51
1:B:90:PRO:HB3	1:B:94:ASP:HB3	1.92	0.50
1:B:212:ASN:HD22	1:B:213:PRO:CD	2.25	0.50
1:B:360:TYR:HB3	1:B:361:PRO:HD2	1.93	0.50
1:A:327:LYS:O	1:A:342:ILE:O	2.29	0.50
1:B:26:LYS:HA	1:B:29:ILE:HG22	1.93	0.49
1:A:4:SER:O	1:A:4:SER:OG	2.25	0.49
1:A:329:MET:HE2	1:A:381:GLN:NE2	2.26	0.49
1:B:212:ASN:HD22	1:B:213:PRO:N	2.11	0.49
1:A:284:THR:HG21	1:A:385:MET:HB2	1.94	0.48
1:A:476:CYS:HB3	1:A:482:PHE:CG	2.48	0.48
1:A:145:ASP:OD2	2:A:2567:GDP:N1	2.45	0.48
1:B:211:ASN:HA	1:B:228:ARG:NH1	2.28	0.48
1:B:130:THR:HG21	1:B:137:ILE:HD11	1.96	0.48
1:A:21:HIS:HD2	1:A:122:ARG:H	1.62	0.47
1:B:369:ASN:HD22	1:B:373:ILE:HG12	1.78	0.47
1:A:11:ALA:O	1:A:14:ARG:NH2	2.48	0.47
1:A:212:ASN:HD22	1:A:212:ASN:C	2.22	0.47
1:B:284:THR:HG21	1:B:385:MET:SD	2.54	0.47
1:A:331:LEU:HD12	1:A:342:ILE:HD12	1.97	0.47
1:A:425:VAL:HG11	1:A:449:VAL:HG21	1.96	0.47
1:B:342:ILE:HD13	1:B:367:LEU:HD22	1.97	0.47
1:A:278:ALA:HB1	1:A:279:PRO:HD2	1.96	0.46
1:A:10:VAL:HG22	1:A:361:PRO:HG2	1.98	0.46
1:B:110:LEU:HD22	1:B:268:MET:HE2	1.97	0.46
1:B:219:VAL:O	1:B:219:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:HD2	1:A:262:ASN:HB2	1.97	0.46
1:B:289:VAL:HG11	1:B:297:THR:HG21	1.97	0.46
1:A:360:TYR:HB3	1:A:361:PRO:HD2	1.97	0.45
1:B:278:ALA:O	1:B:279:PRO:C	2.59	0.45
1:A:453:LEU:O	1:A:457:TYR:O	2.33	0.45
1:B:18:ILE:HG12	1:B:110:LEU:HD23	1.99	0.45
1:A:496:ASP:HB3	1:A:498:GLY:H	1.81	0.45
1:A:375:ILE:CG2	1:A:390:ILE:HD11	2.47	0.45
1:B:212:ASN:HD22	1:B:213:PRO:HD2	1.81	0.45
1:B:29:ILE:CD1	1:B:265:VAL:HG22	2.47	0.45
1:B:496:ASP:HB3	1:B:498:GLY:H	1.82	0.44
1:B:145:ASP:OD2	2:B:3567:GDP:N1	2.45	0.44
1:B:416:LEU:HB3	1:B:427:VAL:HG11	1.99	0.44
1:A:405:ASP:OD2	1:A:406:PRO:HA	2.18	0.44
1:B:278:ALA:HB1	1:B:279:PRO:HD2	1.99	0.44
1:B:391:PRO:HG2	1:B:393:PHE:CZ	2.53	0.44
1:A:170:THR:HA	1:A:183:TYR:O	2.17	0.43
1:B:296:PHE:HZ	1:B:318:MET:HE3	1.82	0.43
1:A:289:VAL:HG11	1:A:297:THR:HG21	1.99	0.43
1:B:21:HIS:HD2	1:B:122:ARG:H	1.65	0.43
1:A:405:ASP:CB	1:A:406:PRO:CA	2.92	0.43
1:A:191:TYR:CD1	1:A:267:HIS:CE1	3.07	0.43
1:A:416:LEU:HB3	1:A:427:VAL:HG11	2.00	0.43
1:B:32:LYS:HA	1:B:32:LYS:HD3	1.88	0.43
1:A:101:ARG:HD2	1:A:390:ILE:CD1	2.50	0.42
1:B:294:ASP:O	1:B:295:LYS:O	2.37	0.42
1:B:425:VAL:HG12	1:B:445:GLN:HB3	2.01	0.42
1:A:401:ILE:HD13	1:A:401:ILE:HA	1.91	0.42
1:A:284:THR:CG2	1:A:285:ASP:N	2.82	0.42
1:B:401:ILE:CD1	1:B:461:ALA:HB1	2.49	0.42
1:A:212:ASN:ND2	1:A:214:ASP:H	2.16	0.42
1:B:9:GLU:O	1:B:13:ARG:HG2	2.19	0.42
1:B:212:ASN:HD22	1:B:212:ASN:C	2.27	0.42
1:A:313:ASP:O	1:A:314:ARG:C	2.63	0.41
1:A:401:ILE:HG12	1:A:463:TYR:HE2	1.86	0.41
1:B:284:THR:CG2	1:B:385:MET:HB2	2.51	0.41
1:A:284:THR:HG22	1:A:286:THR:N	2.35	0.41
1:B:157:GLU:O	1:B:161:GLU:HB2	2.21	0.41
1:A:16:PHE:CZ	1:A:86:LEU:HD13	2.56	0.41
1:B:95:PHE:CE2	1:B:122:ARG:NH2	2.89	0.41
1:B:167:ALA:O	1:B:253:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PRO:HD3	1:A:256:PHE:CG	2.56	0.41
1:A:216:ASP:HB3	1:A:221:GLU:HG3	2.03	0.41
1:B:476:CYS:HB3	1:B:482:PHE:CG	2.56	0.41
1:A:297:THR:HB	1:A:322:SER:OG	2.21	0.41
1:B:101:ARG:HD2	1:B:390:ILE:CD1	2.51	0.41
1:A:278:ALA:O	1:A:279:PRO:C	2.65	0.40
1:A:399:ARG:HA	1:A:466:VAL:HG22	2.03	0.40
1:A:284:THR:HG22	1:A:285:ASP:N	2.35	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	480/529 (91%)	449 (94%)	22 (5%)	9 (2%)	6	22
1	B	469/529 (89%)	433 (92%)	32 (7%)	4 (1%)	14	41
All	All	949/1058 (90%)	882 (93%)	54 (6%)	13 (1%)	9	30

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	295	LYS
1	A	309	PRO
1	A	405	ASP
1	B	294	ASP
1	B	295	LYS
1	B	315	VAL
1	A	294	ASP
1	A	306	ASN
1	A	308	ASP

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Mol	Chain	Res	Type
1	B	92	HIS
1	A	391	PRO
1	A	425	VAL

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	420/453 (93%)	374 (89%)	46 (11%)	6	20
1	B	411/453 (91%)	366 (89%)	45 (11%)	6	21
All	All	831/906 (92%)	740 (89%)	91 (11%)	6	20

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	4	SER
1	A	8	GLN
1	A	14	ARG
1	A	33	VAL
1	A	35	LEU
1	A	74	VAL
1	A	75	MET
1	A	87	LEU
1	A	117	LYS
1	A	122	ARG
1	A	130	THR
1	A	155	LEU
1	A	156	ASP
1	A	169	ILE
1	A	178	LEU
1	A	192	LEU
1	A	197	LYS
1	A	231	LEU
1	A	258	THR

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Mol	Chain	Res	Type
1	A	268	MET
1	A	273	VAL
1	A	284	THR
1	A	286	THR
1	A	294	ASP
1	A	297	THR
1	A	332	ARG
1	A	347	THR
1	A	356	VAL
1	A	365	LEU
1	A	369	ASN
1	A	390	ILE
1	A	392	ASN
1	A	397	LEU
1	A	399	ARG
1	A	401	ILE
1	A	403	LEU
1	A	404	LYS
1	A	410	LYS
1	A	427	VAL
1	A	458	ASN
1	A	467	ASN
1	A	474	VAL
1	A	481	LYS
1	A	506	THR
1	A	516	GLU
1	B	3	LEU
1	B	14	ARG
1	B	23	ASP
1	B	35	LEU
1	B	74	VAL
1	B	75	MET
1	B	87	LEU
1	B	94	ASP
1	B	117	LYS
1	B	122	ARG
1	B	130	THR
1	B	155	LEU
1	B	156	ASP
1	B	178	LEU
1	B	192	LEU
1	B	197	LYS

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Mol	Chain	Res	Type
1	B	231	LEU
1	B	258	THR
1	B	268	MET
1	B	284	THR
1	B	297	THR
1	B	332	ARG
1	B	347	THR
1	B	369	ASN
1	B	372	THR
1	B	390	ILE
1	B	392	ASN
1	B	396	GLU
1	B	397	LEU
1	B	399	ARG
1	B	401	ILE
1	B	403	LEU
1	B	404	LYS
1	B	410	LYS
1	B	427	VAL
1	B	456	GLU
1	B	458	ASN
1	B	459	VAL
1	B	470	THR
1	B	481	LYS
1	B	496	ASP
1	B	499	ASP
1	B	506	THR
1	B	516	GLU
1	B	525	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	21	HIS
1	A	85	ASN
1	A	160	ASN
1	A	184	HIS
1	A	202	GLN
1	A	211	ASN
1	A	212	ASN
1	A	262	ASN

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Mol	Chain	Res	Type
1	A	369	ASN
1	A	392	ASN
1	A	458	ASN
1	A	500	ASN
1	B	8	GLN
1	B	21	HIS
1	B	76	GLN
1	B	92	HIS
1	B	202	GLN
1	B	212	ASN
1	B	262	ASN
1	B	267	HIS
1	B	369	ASN
1	B	392	ASN
1	B	458	ASN
1	B	500	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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
2	GDP	A	2567	-	29,30,30	0.84	0	45,47,47	1.46	7 (15%)
2	GDP	B	3567	-	29,30,30	0.98	1 (3%)	45,47,47	1.50	8 (17%)

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
2	GDP	A	2567	-	-	0/16/32/32	0/3/3/3
2	GDP	B	3567	-	-	2/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3567	GDP	PA-O3A	3.21	1.63	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3567	GDP	C5-C4-N3	-4.20	121.71	128.39
2	A	2567	GDP	C5-C4-N3	-4.14	121.80	128.39
2	A	2567	GDP	C2-N3-C4	3.90	119.01	112.30
2	B	3567	GDP	C2-N3-C4	3.84	118.92	112.30
2	A	2567	GDP	N9-C8-N7	-2.61	108.56	113.40
2	A	2567	GDP	N9-C4-N3	2.61	131.16	125.95
2	B	3567	GDP	N9-C8-N7	-2.60	108.58	113.40
2	B	3567	GDP	N9-C4-N3	2.45	130.86	125.95
2	B	3567	GDP	C2-N1-C6	-2.42	120.72	125.11
2	A	2567	GDP	O6-C6-C5	-2.40	120.19	126.53
2	A	2567	GDP	C8-N7-C5	2.32	108.39	104.26
2	B	3567	GDP	C5-C6-N1	2.23	118.92	113.25
2	B	3567	GDP	O2B-PB-O3A	2.17	111.93	104.64
2	A	2567	GDP	C2-N1-C6	-2.17	121.17	125.11
2	B	3567	GDP	C8-N7-C5	2.10	107.99	104.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3567	GDP	PA-O3A-PB-O3B

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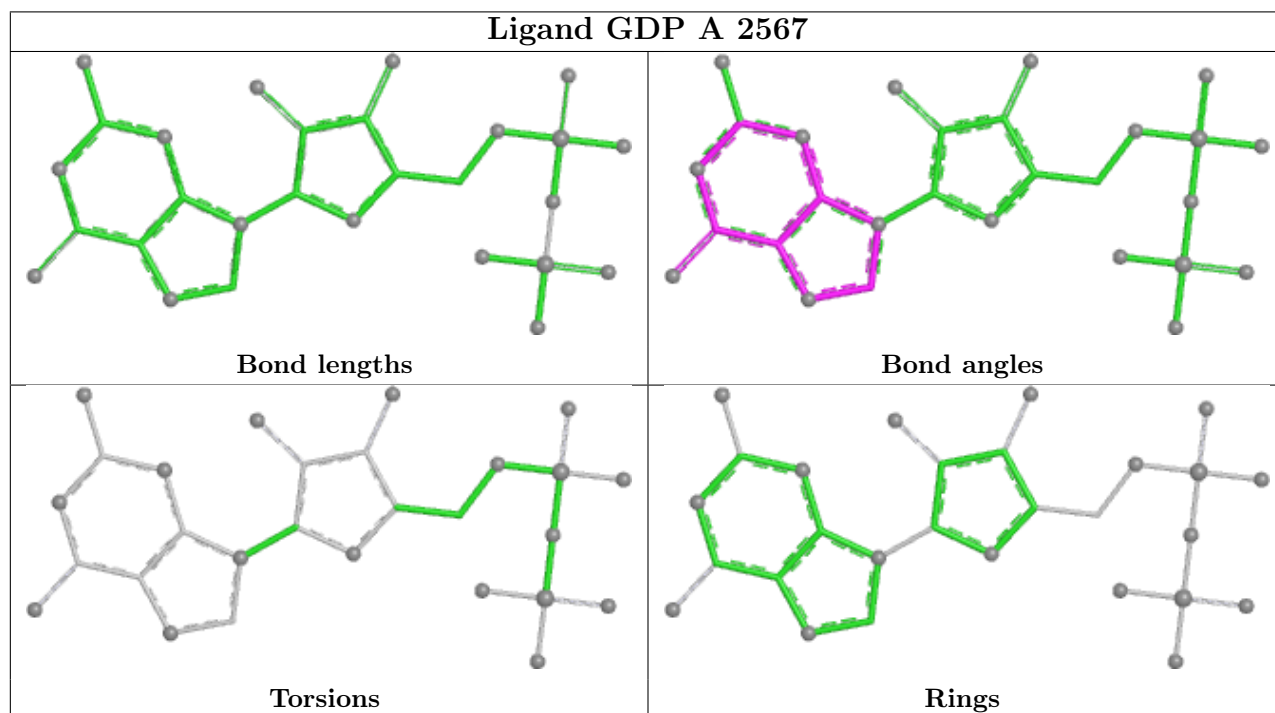
Mol	Chain	Res	Type	Atoms
2	B	3567	GDP	PA-O3A-PB-O2B

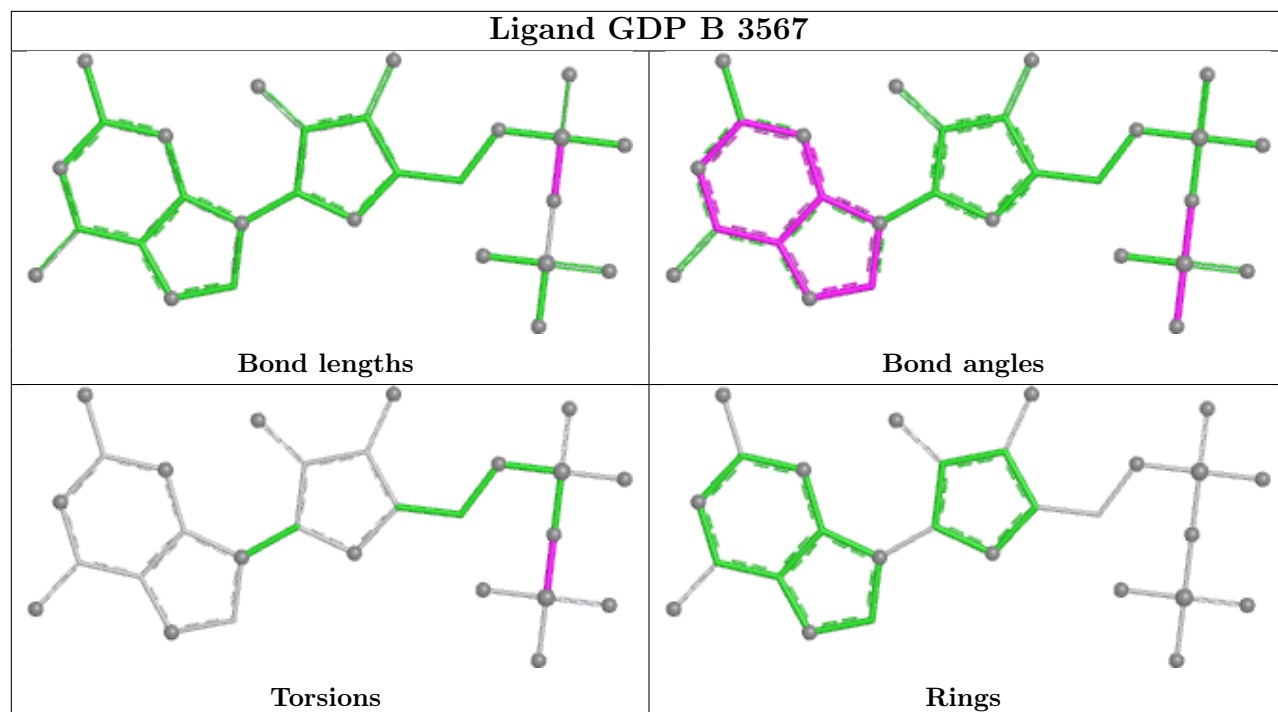
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2567	GDP	1	0
2	B	3567	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	488/529 (92%)	-0.11	16 (3%)	49	39	14, 30, 51, 65	0
1	B	479/529 (90%)	0.28	20 (4%)	40	32	23, 42, 63, 71	0
All	All	967/1058 (91%)	0.08	36 (3%)	45	36	14, 35, 59, 71	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	ASP	4.0
1	B	370	HIS	3.8
1	B	2	THR	3.8
1	B	305	ALA	3.6
1	A	71	THR	3.6
1	B	71	THR	3.5
1	B	3	LEU	3.4
1	B	314	ARG	3.4
1	A	356	VAL	3.2
1	B	356	VAL	2.9
1	B	344	ASP	2.9
1	A	70	ILE	2.8
1	A	309	PRO	2.8
1	A	202	GLN	2.7
1	A	3	LEU	2.7
1	B	403	LEU	2.7
1	B	359	ALA	2.6
1	B	422	GLU	2.5
1	A	305	ALA	2.4
1	A	458	ASN	2.4
1	B	481	LYS	2.4
1	A	404	LYS	2.3
1	B	434	ASN	2.3
1	B	72	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	145	ASP	2.3
1	B	315	VAL	2.3
1	A	314	ARG	2.3
1	B	357	GLU	2.2
1	B	417	VAL	2.2
1	A	294	ASP	2.1
1	B	343	SER	2.1
1	A	406	PRO	2.1
1	A	344	ASP	2.0
1	A	311	HIS	2.0
1	B	225	GLN	2.0
1	A	410	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

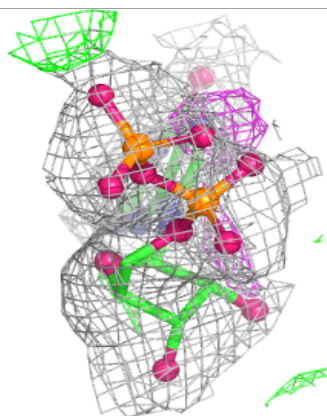
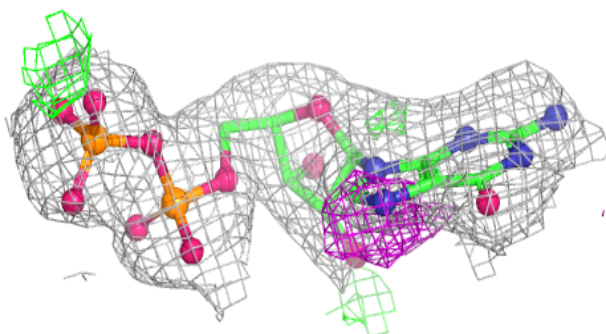
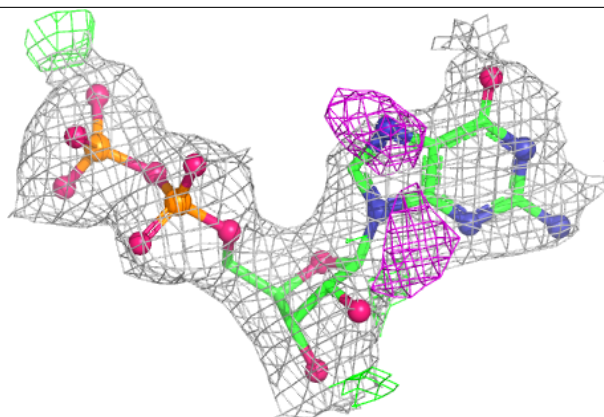
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GDP	B	3567	28/28	0.94	0.10	21,25,27,27	0
2	GDP	A	2567	28/28	0.96	0.08	21,26,28,30	0

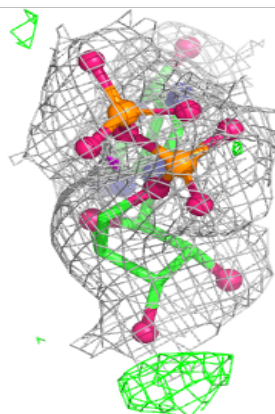
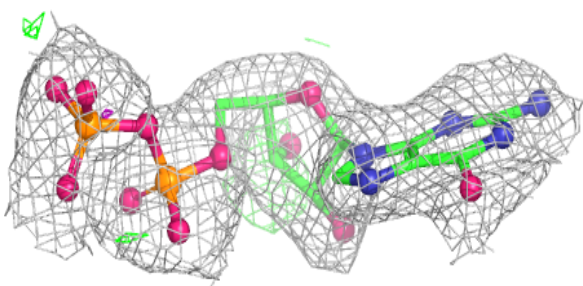
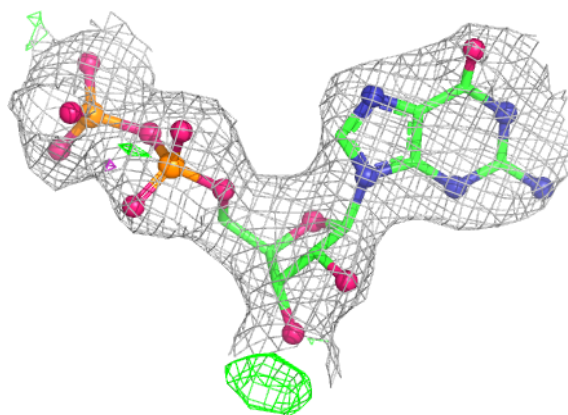
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP B 3567:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GDP A 2567:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.