



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:49 PM UTC

PDB ID : 1D5T / pdb_00001d5t
Title : GUANINE NUCLEOTIDE DISSOCIATION INHIBITOR, ALPHA-ISOFORM
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Deposited on : 1999-10-11
Resolution : 1.04 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

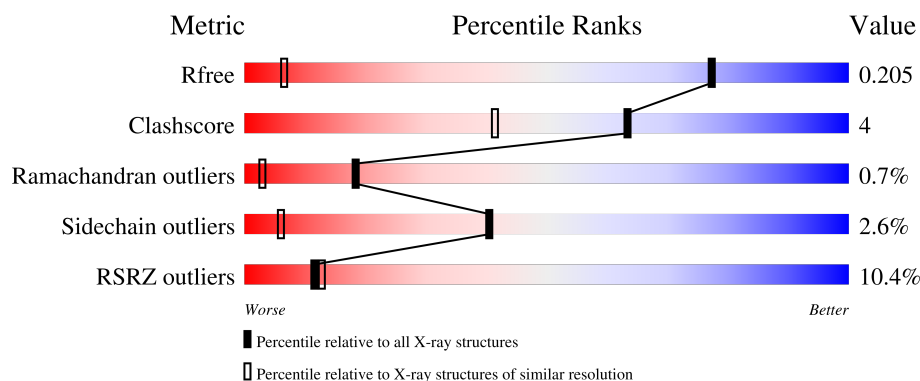
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.04 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	1036 (1.06-1.02)
Clashscore	190562	1063 (1.06-1.02)
Ramachandran outliers	187476	1034 (1.06-1.02)
Sidechain outliers	187428	1035 (1.06-1.02)
RSRZ outliers	180081	1035 (1.06-1.02)

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	433	10% 84% 13% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3827 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 GUANINE NUCLEOTIDE DISSOCIATION INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	433	3430	2182	564	658	26	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	HIS	-	conflict	UNP P21856
A	-1	HIS	-	conflict	UNP P21856

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

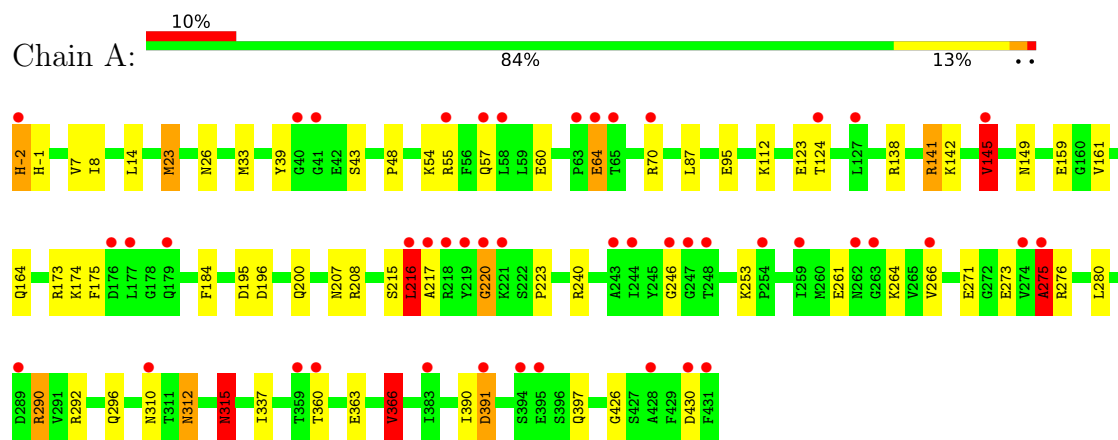
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	387	Total 387	O 387	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: GUANINE NUCLEOTIDE DISSOCIATION INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.29Å 42.74Å 61.78Å 90.00° 104.55° 90.00°	Depositor
Resolution (Å)	10.00 – 1.04 10.00 – 1.04	Depositor EDS
% Data completeness (in resolution range)	91.0 (10.00-1.04) 92.0 (10.00-1.04)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.04Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.173 , 0.209 0.175 , 0.205	Depositor DCC
R_{free} test set	10372 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 53.9	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	0.95	EDS
Total number of atoms	3827	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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: SO4

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	1.37	4/3513 (0.1%)	1.76	73/4752 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	ALA	C-O	59.99	1.95	1.23
1	A	275	ALA	C-N	-8.97	1.21	1.33
1	A	208	ARG	CD-NE	-7.26	1.36	1.46
1	A	95	GLU	C-N	-5.49	1.28	1.34

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	LEU	CA-C-N	29.35	177.61	121.54
1	A	216	LEU	C-N-CA	29.35	177.61	121.54
1	A	275	ALA	O-C-N	-20.03	98.23	122.87
1	A	275	ALA	CA-C-O	-15.86	103.72	120.84
1	A	208	ARG	CD-NE-CZ	15.50	146.10	124.40
1	A	360	THR	CA-C-N	14.27	141.75	123.34
1	A	360	THR	C-N-CA	14.27	141.75	123.34
1	A	39	TYR	CA-C-N	13.61	143.87	122.51
1	A	39	TYR	C-N-CA	13.61	143.87	122.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	ALA	CA-C-N	13.35	141.90	120.94
1	A	275	ALA	C-N-CA	13.35	141.90	120.94
1	A	26	ASN	OD1-CG-ND2	-13.00	109.60	122.60
1	A	138	ARG	CD-NE-CZ	12.71	142.19	124.40
1	A	124	THR	CA-C-N	10.13	134.27	120.38
1	A	124	THR	C-N-CA	10.13	134.27	120.38
1	A	246	GLY	CA-C-N	-9.80	115.17	122.33
1	A	246	GLY	C-N-CA	-9.80	115.17	122.33
1	A	23	MET	CG-SD-CE	9.74	122.34	100.90
1	A	39	TYR	O-C-N	-9.61	111.44	122.68
1	A	366	VAL	CA-CB-CG2	-9.04	95.04	110.40
1	A	195	ASP	O-C-N	-8.91	111.39	122.35
1	A	60	GLU	CB-CG-CD	8.64	127.28	112.60
1	A	124	THR	O-C-N	-8.55	113.26	122.07
1	A	26	ASN	CA-CB-CG	8.53	121.12	112.60
1	A	145	VAL	CA-CB-CG1	8.19	124.31	110.40
1	A	195	ASP	CA-C-N	7.89	131.19	120.38
1	A	195	ASP	C-N-CA	7.89	131.19	120.38
1	A	391	ASP	CA-C-O	-7.82	111.94	120.30
1	A	292	ARG	CD-NE-CZ	7.62	135.07	124.40
1	A	149	ASN	CB-CG-ND2	7.54	127.70	116.40
1	A	315	ASN	OD1-CG-ND2	-7.44	115.16	122.60
1	A	315	ASN	CA-CB-CG	7.32	119.92	112.60
1	A	-2	HIS	CA-CB-CG	6.97	120.77	113.80
1	A	223	PRO	CA-C-N	6.93	132.97	122.65
1	A	223	PRO	C-N-CA	6.93	132.97	122.65
1	A	14	LEU	CA-C-N	6.87	129.37	120.44
1	A	14	LEU	C-N-CA	6.87	129.37	120.44
1	A	290	ARG	CD-NE-CZ	6.56	133.59	124.40
1	A	26	ASN	CB-CG-OD1	6.47	133.73	120.80
1	A	184	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	141	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	A	310	ASN	CA-CB-CG	-6.18	106.42	112.60
1	A	220	GLY	CA-C-N	-6.01	112.00	122.64
1	A	220	GLY	C-N-CA	-6.01	112.00	122.64
1	A	64	GLU	CA-C-O	6.00	129.09	120.51
1	A	95	GLU	CA-C-N	5.95	130.52	120.64
1	A	95	GLU	C-N-CA	5.95	130.52	120.64
1	A	138	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	A	112	LYS	CG-CD-CE	5.86	124.77	111.30
1	A	240	ARG	CD-NE-CZ	5.78	132.50	124.40
1	A	196	ASP	CA-CB-CG	5.72	118.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	LYS	O-C-N	-5.69	115.55	123.34
1	A	312	ASN	CB-CG-ND2	5.62	124.83	116.40
1	A	64	GLU	CB-CG-CD	5.58	122.09	112.60
1	A	215	SER	CA-C-N	5.54	132.11	121.54
1	A	215	SER	C-N-CA	5.54	132.11	121.54
1	A	397	GLN	CA-C-N	5.53	130.63	123.11
1	A	397	GLN	C-N-CA	5.53	130.63	123.11
1	A	390	ILE	CA-C-N	5.46	130.70	123.00
1	A	390	ILE	C-N-CA	5.46	130.70	123.00
1	A	208	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	A	207	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	175	PHE	CA-CB-CG	-5.36	108.44	113.80
1	A	391	ASP	CA-CB-CG	5.36	117.95	112.60
1	A	164	GLN	CA-CB-CG	5.32	124.74	114.10
1	A	360	THR	O-C-N	-5.27	115.10	122.37
1	A	57	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	A	14	LEU	O-C-N	-5.17	116.64	122.12
1	A	430	ASP	CA-C-O	5.15	126.28	120.92
1	A	141	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	A	200	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	296	GLN	OE1-CD-NE2	5.03	127.63	122.60
1	A	173	ARG	CD-NE-CZ	5.02	131.43	124.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	LEU	Peptide
1	A	275	ALA	Mainchain

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	3430	0	3385	27	0
2	A	10	0	0	0	0
3	A	387	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3827	0	3385	27	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 4.

All (27) 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:275:ALA:C	1:A:275:ALA:O	1.95	1.10
1:A:-1:HIS:HB3	3:A:1114:HOH:O	1.84	0.76
1:A:363:GLU:O	1:A:366:VAL:HG22	1.86	0.76
1:A:261:GLU:OE1	1:A:266:VAL:HG11	1.88	0.74
1:A:264:LYS:HE2	3:A:1111:HOH:O	1.93	0.69
1:A:271:GLU:HB2	3:A:1166:HOH:O	1.93	0.68
1:A:54:LYS:HD2	3:A:1235:HOH:O	1.96	0.66
1:A:141:ARG:O	1:A:145:VAL:HG13	1.97	0.65
1:A:43:SER:HB2	3:A:1234:HOH:O	1.98	0.63
1:A:8:ILE:O	1:A:280:LEU:HD22	1.99	0.62
1:A:70:ARG:HG2	3:A:1079:HOH:O	2.00	0.61
1:A:264:LYS:HG2	3:A:1111:HOH:O	2.02	0.60
1:A:-1:HIS:HA	1:A:273:GLU:OE1	2.05	0.56
1:A:123:GLU:CD	1:A:145:VAL:HG12	2.31	0.56
1:A:315:ASN:C	1:A:315:ASN:HD22	2.16	0.53
1:A:264:LYS:HE3	3:A:1250:HOH:O	2.12	0.50
1:A:426:GLY:HA2	3:A:1374:HOH:O	2.14	0.48
1:A:48:PRO:HG3	1:A:70:ARG:CZ	2.45	0.47
1:A:275:ALA:O	1:A:276:ARG:N	2.44	0.47
1:A:55:ARG:NH2	3:A:1262:HOH:O	2.48	0.46
1:A:253:LYS:NZ	3:A:1166:HOH:O	2.49	0.46
1:A:290:ARG:NH1	1:A:391:ASP:OD1	2.50	0.45
1:A:142:LYS:O	1:A:145:VAL:HG22	2.17	0.44
1:A:145:VAL:HG22	3:A:1140:HOH:O	2.17	0.44
1:A:159:GLU:O	1:A:174:LYS:HE3	2.18	0.43
1:A:7:VAL:HG21	1:A:23:MET:CE	2.50	0.41
1:A:145:VAL:HG21	3:A:1284:HOH:O	2.21	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	434/433 (100%)	426 (98%)	5 (1%)	3 (1%)	18	3

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	LEU
1	A	217	ALA
1	A	220	GLY

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	381/380 (100%)	370 (97%)	11 (3%)	37	4

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	33[A]	MET
1	A	33[B]	MET
1	A	64	GLU
1	A	87	LEU
1	A	145	VAL
1	A	161	VAL
1	A	312	ASN

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Mol	Chain	Res	Type
1	A	315	ASN
1	A	337	ILE
1	A	366	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	236	GLN
1	A	279	GLN
1	A	315	ASN
1	A	325	GLN

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	SO4	A	502	-	4,4,4	0.42	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	501	-	4,4,4	0.54	0	6,6,6	0.20	0

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	433/433 (100%)	0.81	45 (10%)	11 13	7, 14, 32, 60	3 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	ALA	9.7
1	A	219	TYR	7.2
1	A	247	GLY	6.7
1	A	218	ARG	6.6
1	A	220	GLY	5.4
1	A	216	LEU	5.1
1	A	145	VAL	4.9
1	A	431	PHE	3.7
1	A	58	LEU	3.4
1	A	179	GLN	3.3
1	A	248	THR	3.2
1	A	430	ASP	3.2
1	A	243	ALA	3.1
1	A	63	PRO	2.9
1	A	289	ASP	2.9
1	A	127	LEU	2.8
1	A	310	ASN	2.8
1	A	70	ARG	2.8
1	A	-2	HIS	2.8
1	A	262	ASN	2.8
1	A	360	THR	2.7
1	A	221	LYS	2.7
1	A	244	ILE	2.7
1	A	176	ASP	2.6
1	A	259	ILE	2.6
1	A	65	THR	2.6
1	A	124	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	254	PRO	2.4
1	A	274	VAL	2.4
1	A	246	GLY	2.3
1	A	359	THR	2.3
1	A	428	ALA	2.2
1	A	391	ASP	2.2
1	A	275	ALA	2.2
1	A	177	LEU	2.2
1	A	263	GLY	2.2
1	A	394	SER	2.2
1	A	40	GLY	2.1
1	A	41	GLY	2.1
1	A	383	ILE	2.1
1	A	55	ARG	2.1
1	A	57	GLN	2.1
1	A	64	GLU	2.0
1	A	395	GLU	2.0
1	A	266	VAL	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	SO4	A	501	5/5	0.95	0.09	15,17,23,25	0
2	SO4	A	502	5/5	0.97	0.07	13,13,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.