



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:31 AM UTC

PDB ID : 2GOL / pdb_00002gol
Title : Xray Structure of Gag278
Authors : Kelly, B.N.
Deposited on : 2006-04-13
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

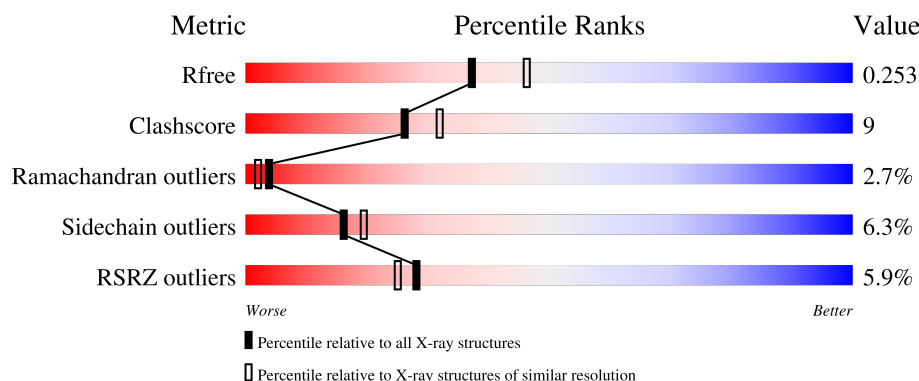
1 Overall quality at a glance

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	133	 2% 48% 24% 5% 23%
2	B	146	 8% 62% 24% • • 8%
2	D	146	 5% 71% 17% • • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3219 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 Matrix protein p17 (MA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	1	0
			825	519	146	158	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	cloning artifact	UNP P12497
A	1	MET	-	cloning artifact	UNP P12497

- Molecule 2 is a protein called Capsid protein p24 (CA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	135	Total	C	N	O	S	0	0	0
			1051	665	185	194	7			
2	D	135	Total	C	N	O	S	0	2	0
			1059	670	186	195	8			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		
4	B	104	Total	O	0	0
			104	104		
4	D	107	Total	O	0	0
			107	107		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.03Å 111.03Å 113.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.81 – 2.20 79.34 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.8 (79.81-2.20) 93.8 (79.34-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.258 0.197 , 0.253	Depositor DCC
R_{free} test set	1703 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k 0.010 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3219	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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	1.48	3/841 (0.4%)	1.29	7/1130 (0.6%)
2	B	1.57	11/1078 (1.0%)	1.46	11/1468 (0.7%)
2	D	1.42	6/1094 (0.5%)	1.30	7/1489 (0.5%)
All	All	1.49	20/3013 (0.7%)	1.36	25/4087 (0.6%)

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
2	B	0	2
2	D	0	1
All	All	0	3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	186	THR	N-CA	10.24	1.58	1.46
2	B	209	ALA	CA-C	8.17	1.63	1.52
1	A	86	TYR	N-CA	-7.07	1.37	1.46
2	B	187	MET	N-CA	6.92	1.54	1.46
2	B	154	ALA	C-O	6.61	1.31	1.24
2	B	153	ASN	C-O	-6.28	1.16	1.24
2	D	217	PRO	CA-C	6.03	1.59	1.52
2	D	216	HIS	N-CA	6.02	1.53	1.46
2	D	249	TRP	N-CA	5.74	1.53	1.46
2	D	258	VAL	CA-CB	5.50	1.62	1.54
2	D	220	ALA	CA-CB	-5.33	1.45	1.53
1	A	48	PRO	N-CA	-5.28	1.40	1.47
2	D	250	MET	SD-CE	-5.21	1.66	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	274	VAL	CA-CB	5.14	1.60	1.54
2	B	188	LEU	CA-CB	5.08	1.61	1.53
2	B	213	ASP	CA-C	5.07	1.59	1.52
1	A	83	ALA	CA-CB	5.06	1.61	1.53
2	B	169	ILE	CA-CB	5.04	1.60	1.54
2	B	190	THR	N-CA	5.03	1.52	1.46
2	B	209	ALA	C-O	-5.00	1.18	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	204	THR	N-CA-C	12.49	137.41	110.80
2	D	225	PRO	N-CA-C	-9.37	96.04	111.68
1	A	70	THR	N-CA-C	-7.32	95.21	110.80
2	B	211	GLU	N-CA-C	7.31	119.25	111.28
2	D	145	GLN	N-CA-C	6.71	119.21	108.41
2	D	224	ALA	N-CA-C	6.66	119.27	110.08
2	B	203	GLU	CB-CA-C	-6.34	100.92	110.88
2	B	205	ILE	N-CA-C	6.29	122.42	109.34
1	A	49	GLY	N-CA-C	-6.27	106.57	114.16
2	B	203	GLU	N-CA-C	6.25	117.76	111.07
1	A	68	LEU	N-CA-C	-6.18	105.22	112.89
2	D	227	GLN	N-CA-C	-6.13	100.57	110.32
2	D	146	ALA	N-CA-C	6.12	123.83	110.80
2	B	232	ARG	CA-C-N	5.81	126.56	119.99
2	B	232	ARG	C-N-CA	5.81	126.56	119.99
2	D	206	ASN	N-CA-C	5.76	117.56	111.28
1	A	73	GLU	N-CA-C	-5.65	105.07	112.41
2	B	163	ALA	N-CA-C	5.62	119.00	111.24
2	B	158	VAL	CB-CA-C	-5.44	104.92	111.88
2	D	226	GLY	N-CA-C	-5.32	97.87	113.30
1	A	78	LEU	N-CA-C	-5.25	105.45	111.07
2	B	223	ILE	N-CA-C	5.25	117.25	109.17
2	B	242	THR	N-CA-CB	-5.21	102.13	110.63
1	A	70	THR	CA-C-N	-5.04	111.53	121.41
1	A	70	THR	C-N-CA	-5.04	111.53	121.41

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	203	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	204	THR	Peptide
2	D	225	PRO	Peptide

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	825	0	839	22	0
2	B	1051	0	1043	18	0
2	D	1059	0	1050	15	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	63	0	0	6	1
4	B	104	0	0	4	1
4	D	107	0	0	7	1
All	All	3219	0	2932	55	2

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 9.

All (55) 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)
2:B:242:THR:HG22	2:B:245:GLU:H	1.10	1.09
2:D:223:ILE:CD1	4:D:316:HOH:O	2.27	0.81
1:A:30:LYS:H	1:A:33:HIS:HD2	1.29	0.78
1:A:30:LYS:H	1:A:33:HIS:CD2	2.02	0.78
1:A:102:ASP:O	1:A:105:GLU:HB2	1.84	0.77
2:B:242:THR:CG2	2:B:245:GLU:H	1.94	0.77
2:B:242:THR:HG22	2:B:245:GLU:N	1.95	0.75
1:A:83:ALA:HB1	1:A:104:ILE:HD13	1.70	0.73
1:A:8:LEU:HD22	1:A:12:GLU:HB3	1.73	0.70
1:A:73:GLU:OE1	4:A:173:HOH:O	2.12	0.68
1:A:69:GLN:C	1:A:70:THR:O	2.29	0.67
2:D:176:SER:OG	2:D:263:LYS:HE3	1.93	0.67
1:A:95:LYS:N	1:A:95:LYS:HD2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:GLN:HG3	4:B:343:HOH:O	1.95	0.65
2:D:186:THR:O	2:D:190:THR:HG23	1.99	0.62
1:A:32:LYS:HA	4:A:180:HOH:O	2.01	0.60
2:D:223:ILE:HD12	4:D:346:HOH:O	2.01	0.60
2:B:167:GLU:HB2	4:B:351:HOH:O	2.02	0.60
2:B:242:THR:HG23	2:B:244:GLN:HG3	1.83	0.59
1:A:40:GLU:OE1	1:A:43:ARG:NH1	2.37	0.58
2:B:162:LYS:HE3	2:B:167:GLU:OE1	2.04	0.57
2:D:223:ILE:HD11	4:D:316:HOH:O	2.00	0.57
2:B:195:GLN:HB2	4:B:310:HOH:O	2.05	0.56
1:A:6:SER:OG	1:A:7:VAL:N	2.38	0.56
2:D:160:GLU:HB3	4:D:385:HOH:O	2.05	0.55
2:D:147:ILE:CG2	2:D:147:ILE:O	2.54	0.54
1:A:32:LYS:CA	4:A:180:HOH:O	2.56	0.53
1:A:50:LEU:HB2	1:A:60:ILE:HD11	1.89	0.53
1:A:30:LYS:N	1:A:33:HIS:HD2	2.03	0.52
2:D:180:THR:HG22	2:D:250:MET:HE1	1.92	0.52
2:B:216:HIS:O	2:B:232:ARG:NH2	2.37	0.51
2:D:153[A]:ASN:ND2	4:D:353:HOH:O	2.45	0.50
2:B:227:GLN:O	2:B:227:GLN:HG3	2.09	0.50
1:A:76:ARG:HD3	4:A:173:HOH:O	2.11	0.50
2:B:146:ALA:O	2:B:147:ILE:C	2.55	0.49
1:A:30:LYS:HB2	1:A:32:LYS:HG2	1.94	0.49
1:A:73:GLU:CD	4:A:173:HOH:O	2.57	0.48
1:A:36:TRP:CZ2	1:A:40:GLU:HG3	2.49	0.48
2:D:169:ILE:N	2:D:170:PRO:HD2	2.29	0.47
1:A:65:GLN:HB3	1:A:66:PRO:HD3	1.96	0.47
1:A:92:ILE:HG21	1:A:103:LYS:HG2	1.97	0.47
2:B:270:LEU:O	2:B:274:VAL:HG13	2.15	0.47
2:D:223:ILE:HD11	4:D:334:HOH:O	2.14	0.46
2:D:246:GLN:C	2:D:250:MET:HE3	2.40	0.46
2:B:244:GLN:CG	4:B:343:HOH:O	2.58	0.46
1:A:32:LYS:CB	4:A:180:HOH:O	2.63	0.46
2:B:167:GLU:O	2:B:170:PRO:HD2	2.16	0.46
2:D:147:ILE:O	2:D:147:ILE:HG23	2.16	0.45
2:B:198:MET:O	2:B:202:LYS:HG3	2.18	0.43
1:A:20:ARG:O	1:A:96:ASP:HA	2.20	0.42
2:B:165:SER:O	2:B:168:VAL:HG12	2.19	0.41
2:B:201:LEU:HB2	2:B:273:ILE:HD11	2.03	0.41
2:B:253:ASN:HA	2:B:254:PRO:HA	1.70	0.40
2:D:270:LEU:O	2:D:274:VAL:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:252:HIS:HE1	4:D:310:HOH:O	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:187:HOH:O	4:B:357:HOH:O[7_555]	1.96	0.24
4:D:363:HOH:O	4:D:363:HOH:O[7_555]	2.15	0.05

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	101/133 (76%)	96 (95%)	5 (5%)	0	100	100
2	B	133/146 (91%)	120 (90%)	6 (4%)	7 (5%)	1	0
2	D	135/146 (92%)	127 (94%)	5 (4%)	3 (2%)	5	3
All	All	369/425 (87%)	343 (93%)	16 (4%)	10 (3%)	4	2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	204	THR
2	B	205	ILE
2	B	222	PRO
2	B	225	PRO
2	D	163	ALA
2	D	146	ALA
2	D	147	ILE
2	B	221	GLY
2	B	227	GLN
2	B	228	MET

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	91/113 (80%)	82 (90%)	9 (10%)	7	8
2	B	113/123 (92%)	107 (95%)	6 (5%)	20	26
2	D	115/123 (94%)	110 (96%)	5 (4%)	26	35
All	All	319/359 (89%)	299 (94%)	20 (6%)	16	19

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	26	LYS
1	A	65	GLN
1	A	75	LEU
1	A	77	SER
1	A	93	ASP
1	A	95	LYS
1	A	104	ILE
1	A	106	GLU
2	B	195	GLN
2	B	242	THR
2	B	244	GLN
2	B	268	LEU
2	B	274	VAL
2	B	275	ARG
2	D	147	ILE
2	D	152	LEU
2	D	223	ILE
2	D	272	LYS
2	D	274	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	33	HIS

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Mol	Chain	Res	Type
1	A	69	GLN
1	A	80	ASN
2	B	206	ASN
2	D	216	HIS

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	$\# Z > 2$
3	SO4	D	2	-	4,4,4	0.69	0	6,6,6	2.16	3 (50%)
3	SO4	A	133	-	4,4,4	0.17	0	6,6,6	0.73	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	SO4	O4-S-O1	-3.35	92.04	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	SO4	O4-S-O2	2.54	122.84	109.56
3	D	2	SO4	O3-S-O2	-2.11	98.51	109.56

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	102/133 (76%)	0.36	3 (2%) 53 50	26, 49, 68, 92	1 (0%)
2	B	135/146 (92%)	0.23	12 (8%) 15 13	27, 42, 88, 101	0
2	D	135/146 (92%)	0.16	7 (5%) 33 29	28, 45, 73, 86	2 (1%)
All	All	372/425 (87%)	0.24	22 (5%) 28 25	26, 45, 78, 101	3 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	224	ALA	4.9
2	B	225	PRO	4.6
2	D	144	HIS	4.5
2	D	145	GLN	4.3
2	B	223	ILE	4.2
2	B	226	GLY	4.0
1	A	6	SER	3.8
2	B	222	PRO	3.8
2	D	146	ALA	3.1
2	D	276	MET	3.0
2	D	277	TYR	2.7
1	A	104	ILE	2.6
2	D	163	ALA	2.5
2	B	144	HIS	2.5
2	B	244	GLN	2.5
2	D	164	PHE	2.3
2	B	254	PRO	2.3
2	B	164	PHE	2.2
2	B	220	ALA	2.2
1	A	26	LYS	2.1
2	B	219	HIS	2.1
2	B	218	VAL	2.1

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
3	SO4	D	2	5/5	0.92	0.14	41,50,56,57	0
3	SO4	A	133	5/5	0.94	0.10	57,57,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.