



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:42 AM UTC

PDB ID : 8DUZ / pdb_00008duz
Title : Protective antibody against gonococcal lipooligosaccharide bound to peptide mimetic
Authors : Beernink, P.T.; Beernink, B.P.; Rice, P.A.; Ram, S.
Deposited on : 2022-07-27
Resolution : 1.65 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

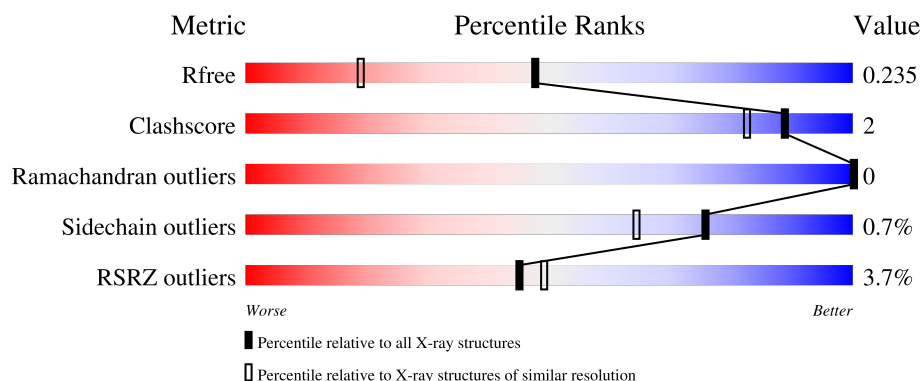
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	221	5% 90% 5%
1	C	221	4% 87% 7% 6%
2	B	215	% 94% ..
2	D	215	3% 94% ..
3	E	17	6% 65% 35%

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Mol	Chain	Length	Quality of chain
3	F	17	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13580 atoms, of which 6408 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 IgG heavy chain, Fd fragment.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	209	Total	C	H	N	O	S	0	1	0
			3136	1009	1542	263	316	6			
1	C	208	Total	C	H	N	O	S	0	2	0
			3132	1008	1540	262	314	8			

- Molecule 2 is a protein called Ig, lambda light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	211	Total	C	H	N	O	S	0	2	0
			3133	1001	1547	264	316	5			
2	B	211	Total	C	H	N	O	S	0	6	0
			3170	1015	1566	263	321	5			

- Molecule 3 is a protein called Mimetic peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	11	Total	C	H	N	O	0	0	0
			160	54	78	12	16			
3	F	15	Total	C	H	N	O	0	0	0
			214	72	106	16	20			

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

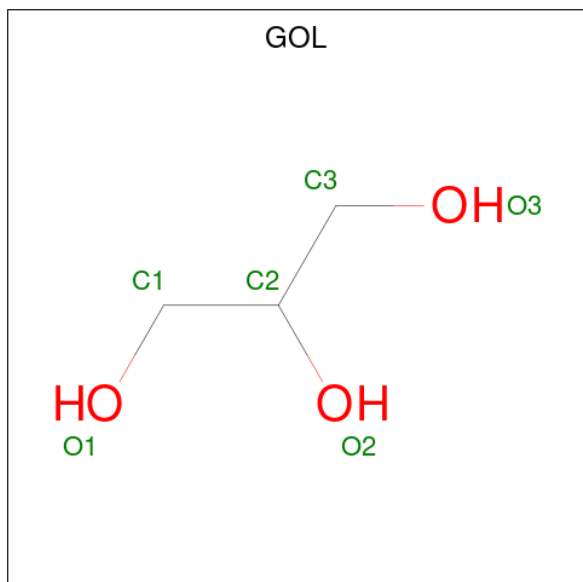


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	B	1	Total	C	H	O	0	0
			7	2	3	2		

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

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C H O 13 3 7 3	0	0
6	C	1	Total C H O 14 3 8 3	0	0
6	C	1	Total C H O 14 3 8 3	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Na 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	146	Total O 146 146	0	0
8	C	111	Total O 111 111	0	0
8	D	142	Total O 142 142	0	0
8	B	172	Total O 172 172	0	0
8	E	3	Total O 3 3	0	0
8	F	4	Total O 4 4	0	0

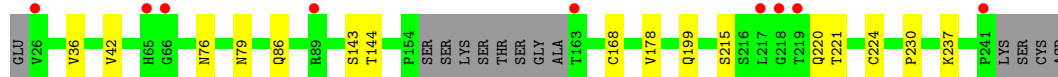
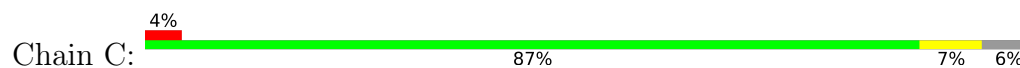
3 Residue-property plots [i](#)

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.

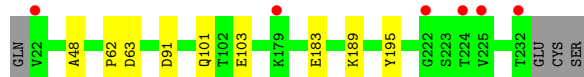
- Molecule 1: IgG heavy chain, Fd fragment



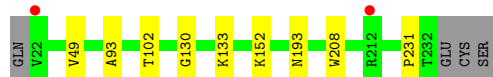
- Molecule 1: IgG heavy chain, Fd fragment



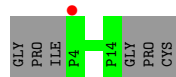
- Molecule 2: Ig, lambda light chain



- Molecule 2: Ig, lambda light chain

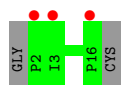


- Molecule 3: Mimetic peptide



- Molecule 3: Mimetic peptide

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.61Å 64.19Å 110.81Å 90.00° 97.12° 90.00°	Depositor
Resolution (Å)	58.16 – 1.65 58.16 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.4 (58.16-1.65) 89.7 (58.16-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.35 (at 1.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.189 , 0.234 0.190 , 0.235	Depositor DCC
R_{free} test set	1894 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13580	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0786e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CL, NA, GOL

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	0.46	0/1638	0.59	0/2234
1	C	0.48	0/1639	0.62	0/2235
2	B	0.51	0/1661	0.62	0/2275
2	D	0.51	0/1631	0.66	0/2234
3	E	0.37	0/84	0.65	0/114
3	F	0.42	0/112	0.58	0/154
All	All	0.49	0/6765	0.62	0/9246

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1594	1542	1543	5	0
1	C	1592	1540	1543	10	0
2	B	1604	1566	1578	6	0
2	D	1586	1547	1551	5	0
3	E	82	78	78	0	0
3	F	108	106	106	0	0
4	A	4	3	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	3	3	0	0
5	A	1	0	0	0	0
6	C	18	23	24	0	0
7	B	1	0	0	0	0
8	A	146	0	0	0	1
8	B	172	0	0	2	2
8	C	111	0	0	1	0
8	D	142	0	0	0	1
8	E	3	0	0	0	0
8	F	4	0	0	0	0
All	All	7172	6408	6429	25	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 2.

All (25) 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:149:VAL:H	4:A:301:ACT:H2	1.51	0.73
2:B:102[A]:THR:HG22	2:B:130:GLY:HA3	1.87	0.57
1:C:199:GLN:HG3	8:C:429:HOH:O	2.12	0.50
1:C:36:VAL:HG11	1:C:42:VAL:CG1	2.42	0.49
1:A:212:VAL:HB	1:A:213:PRO:HD2	1.99	0.45
2:D:189:LYS:HE2	2:D:195:TYR:OH	2.17	0.45
1:A:26:VAL:HG11	1:A:130:TYR:CD1	2.51	0.45
2:B:193:ASN:HB2	8:B:402:HOH:O	2.17	0.44
1:C:168[B]:CYS:SG	1:C:224[B]:CYS:SG	3.15	0.44
1:C:168[B]:CYS:CB	1:C:224[B]:CYS:HG	2.30	0.44
2:D:48:ALA:HA	2:D:91:ASP:HB2	1.99	0.44
1:C:220:GLN:HG3	1:C:221:THR:N	2.33	0.44
2:D:62:PRO:O	2:D:63:ASP:HB2	2.18	0.44
1:A:206:LEU:HD12	1:A:206:LEU:C	2.43	0.43
1:C:224[B]:CYS:SG	1:C:237:LYS:HB3	2.58	0.43
1:C:144:THR:HG21	1:C:230:PRO:O	2.17	0.43
1:C:199:GLN:OE1	2:D:183:GLU:HG3	2.19	0.42
2:B:133:LYS:NZ	8:B:403:HOH:O	2.50	0.42
1:C:144:THR:HG21	1:C:230:PRO:C	2.44	0.42
2:B:152:LYS:HD3	2:B:152:LYS:HA	1.83	0.42
1:A:77:PRO:HB3	1:A:96:VAL:HG21	2.02	0.41
1:C:76:ASN:HB3	1:C:79:ASN:OD1	2.20	0.41
2:D:101[B]:GLN:OE1	2:D:103:GLU:OE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:VAL:HG11	2:B:93:ALA:HB2	2.03	0.41
2:B:208:TRP:CZ2	2:B:231:PRO:HA	2.57	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)
8:D:426:HOH:O	8:B:492:HOH:O[2_545]	2.12	0.08
8:A:484:HOH:O	8:B:466:HOH:O[1_655]	2.19	0.01

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	206/221 (93%)	199 (97%)	7 (3%)	0	100	100
1	C	206/221 (93%)	203 (98%)	3 (2%)	0	100	100
2	B	215/215 (100%)	204 (95%)	11 (5%)	0	100	100
2	D	211/215 (98%)	200 (95%)	11 (5%)	0	100	100
3	E	9/17 (53%)	9 (100%)	0	0	100	100
3	F	13/17 (76%)	12 (92%)	1 (8%)	0	100	100
All	All	860/906 (95%)	827 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/192 (95%)	181 (100%)	1 (0%)	81	72
1	C	183/192 (95%)	179 (98%)	4 (2%)	45	23
2	B	180/178 (101%)	180 (100%)	0	100	100
2	D	176/178 (99%)	176 (100%)	0	100	100
3	E	9/13 (69%)	9 (100%)	0	100	100
3	F	12/13 (92%)	12 (100%)	0	100	100
All	All	742/766 (97%)	737 (99%)	5 (1%)	76	64

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

Mol	Chain	Res	Type
1	A	178	VAL
1	C	86	GLN
1	C	143	SER
1	C	178	VAL
1	C	215	SER

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	27	GLN
2	D	75	ASN
2	B	74	ASN
2	B	75	ASN
2	B	211	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
6	GOL	C	303	-	5,5,5	0.86	0	5,5,5	1.23	1 (20%)
4	ACT	B	302	-	3,3,3	1.22	0	3,3,3	1.40	0
4	ACT	A	301	-	3,3,3	1.49	0	3,3,3	1.35	0
6	GOL	C	301	-	5,5,5	0.80	0	5,5,5	0.71	0
6	GOL	C	302	-	5,5,5	1.03	0	5,5,5	1.01	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
6	GOL	C	303	-	-	0/4/4/4	-
6	GOL	C	301	-	-	2/4/4/4	-
6	GOL	C	302	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	303	GOL	C3-C2-C1	-2.09	104.13	111.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	301	GOL	O1-C1-C2-O2
6	C	301	GOL	O1-C1-C2-C3
6	C	302	GOL	C1-C2-C3-O3
6	C	302	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	ACT	1	0

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	209/221 (94%)	0.48	11 (5%) 32 36	23, 36, 57, 88	1 (0%)
1	C	208/221 (94%)	0.54	9 (4%) 40 43	20, 38, 60, 95	2 (0%)
2	B	211/215 (98%)	0.05	2 (0%) 81 86	14, 29, 48, 80	6 (2%)
2	D	211/215 (98%)	0.25	6 (2%) 55 60	18, 32, 52, 72	2 (0%)
3	E	11/17 (64%)	0.86	1 (9%) 15 16	32, 40, 58, 66	0
3	F	15/17 (88%)	0.99	3 (20%) 3 3	27, 40, 65, 82	0
All	All	865/906 (95%)	0.34	32 (3%) 45 49	14, 34, 57, 95	11 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	66	GLY	5.1
3	F	16	PRO	4.2
2	D	179	LYS	3.7
3	E	4	PRO	3.4
2	B	22	VAL	3.1
1	C	65	HIS	3.0
1	C	217	LEU	3.0
2	D	222	GLY	3.0
2	D	225	VAL	2.9
3	F	2	PRO	2.9
2	D	232	THR	2.9
1	C	219	THR	2.8
2	B	212	ARG	2.8
1	A	219	THR	2.8
3	F	3	ILE	2.8
1	C	26	VAL	2.7
1	A	241	PRO	2.6
1	C	163	THR	2.6
1	A	186	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	241	PRO	2.5
1	A	162	ALA	2.5
2	D	224	THR	2.4
1	A	65	HIS	2.4
1	C	218	GLY	2.4
1	A	66	GLY	2.3
1	A	239	VAL	2.3
1	A	217	LEU	2.2
1	A	189	SER	2.1
1	A	218	GLY	2.1
1	C	89	ARG	2.1
1	A	216	SER	2.0
2	D	22	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
4	ACT	B	302	4/4	0.72	0.20	54,59,70,70	0
6	GOL	C	303	6/6	0.76	0.19	61,73,88,88	0
6	GOL	C	302	6/6	0.77	0.17	55,70,77,85	0
4	ACT	A	301	4/4	0.80	0.18	39,47,54,55	0
6	GOL	C	301	6/6	0.80	0.15	54,65,72,86	0
5	CL	A	302	1/1	0.92	0.10	56,56,56,56	0
7	NA	B	301	1/1	0.96	0.06	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.