



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 08:13 PM EDT

PDB ID : 6Q5A
Title : Crystal structure of Cryptosporidium hominis CPSF3 in the apo form
Authors : Palencia, A.; Swale, C.
Deposited on : 2018-12-07
Resolution : 1.55 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

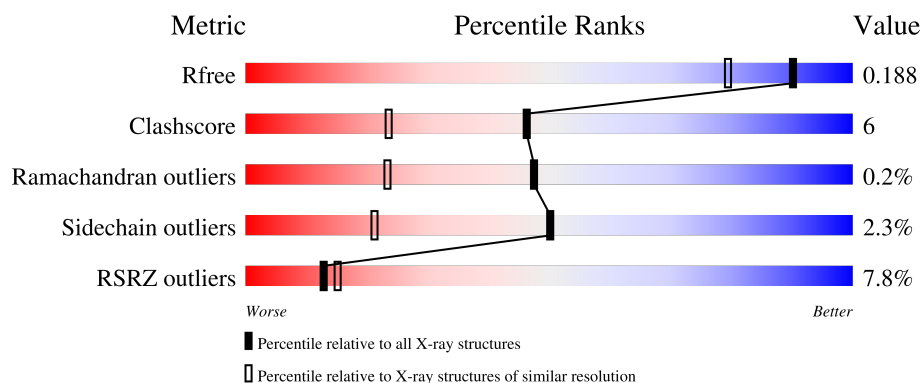
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	483	<div> <div>7%</div> <div>85%</div> <div>9%</div> <div>• 5%</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4245 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 Cleavage and Polyadenylation Specificity Factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	26	0
			3739	2402	625	685	27			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A0S4TJL4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

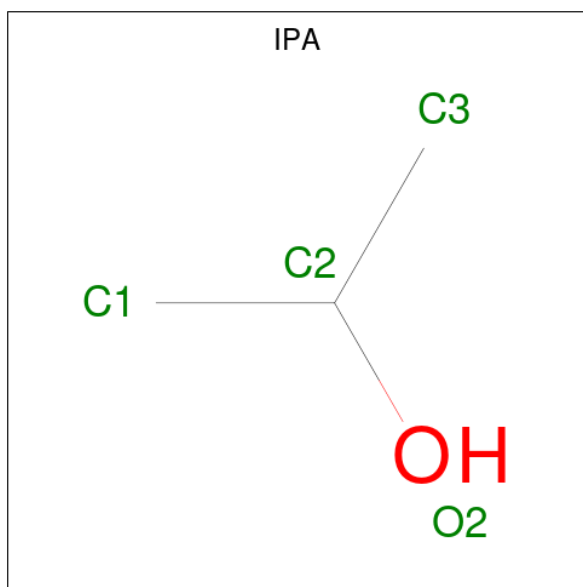
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		
4	A	1	Total	C	O	0	0
			4	3	1		
4	A	1	Total	C	O	0	0
			4	3	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

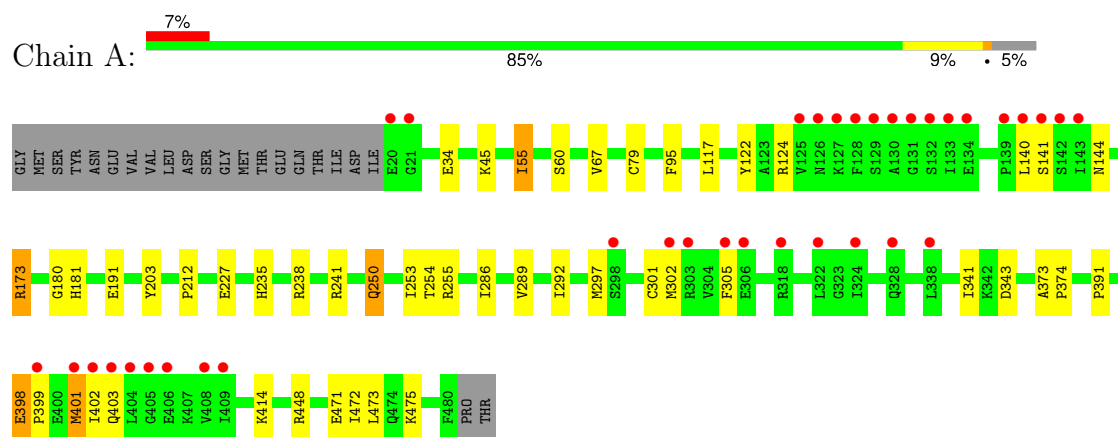
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	471	Total	O	0	0
			471	471		

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: Cleavage and Polyadenylation Specificity Factor 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	90.36Å 90.36Å 238.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.49 – 1.55 47.45 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.49-1.55) 98.0 (47.45-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.138 , 0.179 0.152 , 0.188	Depositor DCC
R_{free} test set	4197 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4245	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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: ZN, MG, GOL, IPA, PG4

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	0.49	0/3889	0.68	0/5262

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	ARG	Sidechain
1	A	241	ARG	Sidechain

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	3739	0	3820	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
3	A	12	0	16	0	0
4	A	12	0	24	4	0
5	A	1	0	0	0	0
6	A	8	0	8	0	0
7	A	471	0	0	8	0
All	All	4245	0	3868	48	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 (48) 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:472[A]:ILE:HG22	1:A:473:LEU:HG	1.37	1.05
1:A:250[A]:GLN:NE2	1:A:286[A]:ILE:HG21	1.86	0.89
1:A:253[B]:ILE:HD12	1:A:286[B]:ILE:HD11	1.65	0.77
1:A:250[A]:GLN:HE21	1:A:286[A]:ILE:HG21	1.47	0.76
1:A:253[B]:ILE:CD1	1:A:286[B]:ILE:HD11	2.16	0.76
1:A:448[A]:ARG:NH2	1:A:471:GLU:OE2	2.16	0.75
1:A:250[A]:GLN:NE2	1:A:286[A]:ILE:CG2	2.49	0.74
1:A:250[A]:GLN:HE21	1:A:286[A]:ILE:CG2	2.04	0.69
1:A:398:GLU:OE1	1:A:398:GLU:N	2.18	0.68
4:A:506:IPA:H11	7:A:665:HOH:O	1.96	0.64
1:A:472[B]:ILE:HG13	7:A:697:HOH:O	1.95	0.64
1:A:235:HIS:O	7:A:601:HOH:O	2.16	0.62
4:A:506:IPA:C1	7:A:665:HOH:O	2.48	0.62
1:A:302:MET:HE3	7:A:907:HOH:O	1.99	0.61
1:A:250[B]:GLN:NE2	1:A:254:THR:OG1	2.30	0.61
1:A:391:PRO:HB3	1:A:403:GLN:HE22	1.65	0.61
1:A:34:GLU:OE2	1:A:472[A]:ILE:HD11	2.01	0.60
1:A:343:ASP:OD2	7:A:602:HOH:O	2.16	0.58
1:A:60:SER:CB	1:A:141:SER:HB3	2.35	0.56
1:A:398:GLU:H	1:A:398:GLU:CD	2.04	0.56
1:A:399:PRO:HD3	7:A:1002:HOH:O	2.06	0.55
1:A:475:LYS:H	4:A:505:IPA:H13	1.71	0.55
1:A:60:SER:HB3	1:A:141:SER:HB3	1.89	0.54
1:A:55[B]:ILE:CD1	1:A:122:TYR:CE1	2.92	0.52
1:A:124:ARG:NH1	1:A:144:ASN:OD1	2.42	0.52
1:A:250[A]:GLN:NE2	1:A:286[A]:ILE:HD13	2.26	0.51
1:A:401:MET:HG3	1:A:403:GLN:HE21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:N	1:A:398:GLU:CD	2.64	0.49
1:A:255:ARG:HH22	1:A:414:LYS:HB3	1.77	0.49
1:A:79[B]:CYS:SG	1:A:95:PHE:HE2	2.36	0.48
1:A:173[B]:ARG:HG3	1:A:191:GLU:HB3	1.96	0.47
1:A:297:MET:HG2	1:A:301[B]:CYS:SG	2.54	0.47
1:A:255:ARG:HH12	1:A:414:LYS:HD2	1.81	0.46
1:A:79[B]:CYS:SG	1:A:95:PHE:CE2	3.09	0.45
1:A:117:LEU:HD13	1:A:301[B]:CYS:SG	2.56	0.45
1:A:301[A]:CYS:SG	1:A:305:PHE:CE1	3.10	0.45
1:A:253[A]:ILE:HG21	1:A:289:VAL:HG21	1.97	0.45
1:A:45:LYS:O	4:A:506:IPA:H33	2.16	0.44
1:A:292:ILE:HG21	1:A:341:ILE:HD13	2.00	0.44
1:A:373:ALA:N	1:A:374:PRO:CD	2.81	0.44
1:A:448[A]:ARG:HH12	1:A:471:GLU:CD	2.18	0.43
1:A:255:ARG:HH22	1:A:414:LYS:CD	2.33	0.42
1:A:255:ARG:NH2	1:A:414:LYS:HB3	2.35	0.42
1:A:399:PRO:CD	7:A:1002:HOH:O	2.65	0.42
1:A:250[A]:GLN:HE22	1:A:286[A]:ILE:HD13	1.85	0.41
1:A:67:VAL:HB	1:A:473:LEU:HD21	2.03	0.40
1:A:250[A]:GLN:NE2	1:A:286[A]:ILE:HG23	2.34	0.40
1:A:180:GLY:HA2	1:A:212:PRO: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	485/483 (100%)	466 (96%)	18 (4%)	1 (0%)	47 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	HIS

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	424/421 (101%)	412 (97%)	12 (3%)	43 14

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55[A]	ILE
1	A	55[B]	ILE
1	A	140	LEU
1	A	173[A]	ARG
1	A	173[B]	ARG
1	A	203	TYR
1	A	227	GLU
1	A	250[A]	GLN
1	A	250[B]	GLN
1	A	398	GLU
1	A	401	MET
1	A	402	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	403	GLN

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	IPA	A	506	-	3,3,3	0.54	0	3,3,3	0.76	0
6	PG4	A	509	-	7,7,12	0.58	0	6,6,11	0.40	0
4	IPA	A	507	-	3,3,3	0.60	0	3,3,3	0.39	0
4	IPA	A	505	-	3,3,3	0.61	0	3,3,3	1.23	0
3	GOL	A	503	-	5,5,5	0.26	0	5,5,5	0.34	0
3	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.66	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	GOL	A	503	-	-	0/4/4/4	-
3	GOL	A	504	-	-	2/4/4/4	-
6	PG4	A	509	-	-	3/5/5/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	GOL	C1-C2-C3-O3
3	A	504	GOL	O2-C2-C3-O3
6	A	509	PG4	C4-C3-O2-C2
6	A	509	PG4	C6-C5-O3-C4
6	A	509	PG4	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506	IPA	3	0
4	A	505	IPA	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	461/483 (95%)	0.11	36 (7%) 13 15	13, 22, 52, 92	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	GLY	8.4
1	A	406	GLU	7.2
1	A	130	ALA	7.1
1	A	128	PHE	6.4
1	A	129	SER	5.2
1	A	399	PRO	5.1
1	A	404	LEU	5.0
1	A	131	GLY	4.9
1	A	140	LEU	4.4
1	A	324	ILE	4.4
1	A	408	VAL	4.3
1	A	127	LYS	3.8
1	A	21	GLY	3.5
1	A	142	SER	3.3
1	A	132	SER	3.0
1	A	133	ILE	3.0
1	A	403	GLN	2.9
1	A	402	ILE	2.9
1	A	143	ILE	2.8
1	A	20	GLU	2.8
1	A	302	MET	2.7
1	A	141	SER	2.7
1	A	134	GLU	2.6
1	A	303	ARG	2.6
1	A	125	VAL	2.6
1	A	409	ILE	2.6
1	A	338	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	298	SER	2.4
1	A	328	GLN	2.3
1	A	305	PHE	2.3
1	A	322	LEU	2.2
1	A	318	ARG	2.2
1	A	139	PRO	2.1
1	A	401	MET	2.1
1	A	306	GLU	2.1
1	A	126	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 monosaccharides 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
6	PG4	A	509	8/13	0.73	0.18	35,47,57,62	0
4	IPA	A	505	4/4	0.85	0.16	22,24,25,41	4
4	IPA	A	506	4/4	0.88	0.12	37,38,40,42	0
3	GOL	A	504	6/6	0.88	0.28	43,44,51,65	0
4	IPA	A	507	4/4	0.93	0.16	28,40,46,49	0
5	MG	A	508	1/1	0.98	0.03	38,38,38,38	0
3	GOL	A	503	6/6	0.98	0.04	23,24,29,30	0
2	ZN	A	502	1/1	1.00	0.05	15,15,15,15	0
2	ZN	A	501	1/1	1.00	0.07	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.