



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:25 PM GMT

PDB ID : 5A99
Title : Crystal structure of Operophtera brumata CPV19 polyhedra
Authors : Ji, X.; Axford, D.; Owen, R.; Evans, G.; Ginn, H.M.; Sutton, G.; Stuart, D.I.
Deposited on : 2015-07-17
Resolution : 1.51 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

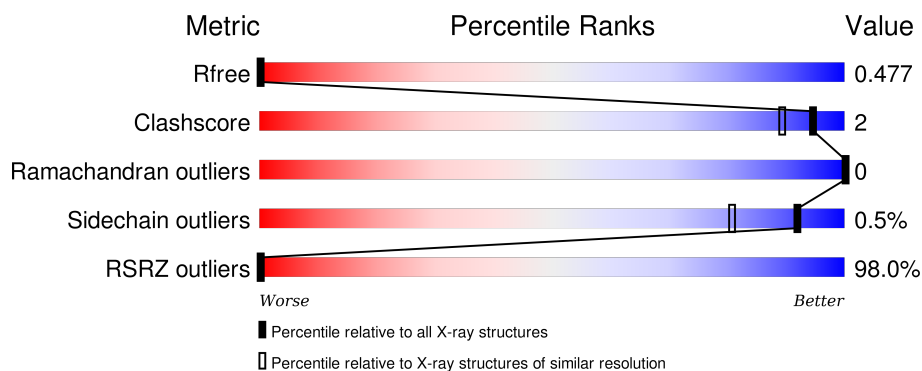
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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}	91344	2658 (1.54-1.50)
Clashscore	102246	2887 (1.54-1.50)
Ramachandran outliers	100387	2818 (1.54-1.50)
Sidechain outliers	100360	2816 (1.54-1.50)
RSRZ outliers	91569	2660 (1.54-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	248	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	A	1250	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	1251	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4301 atoms, of which 1976 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.

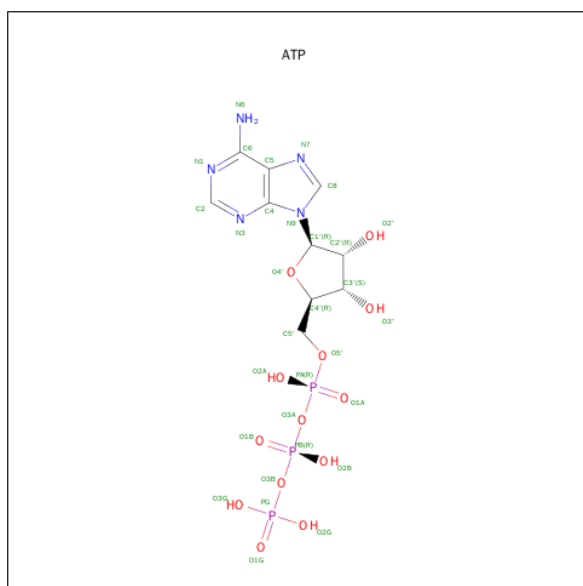
- Molecule 1 is a protein called POLYHEDRIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	248	4022	1300	1964	369	382	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ACE	-	ACETYLATION	UNP Q30C66

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

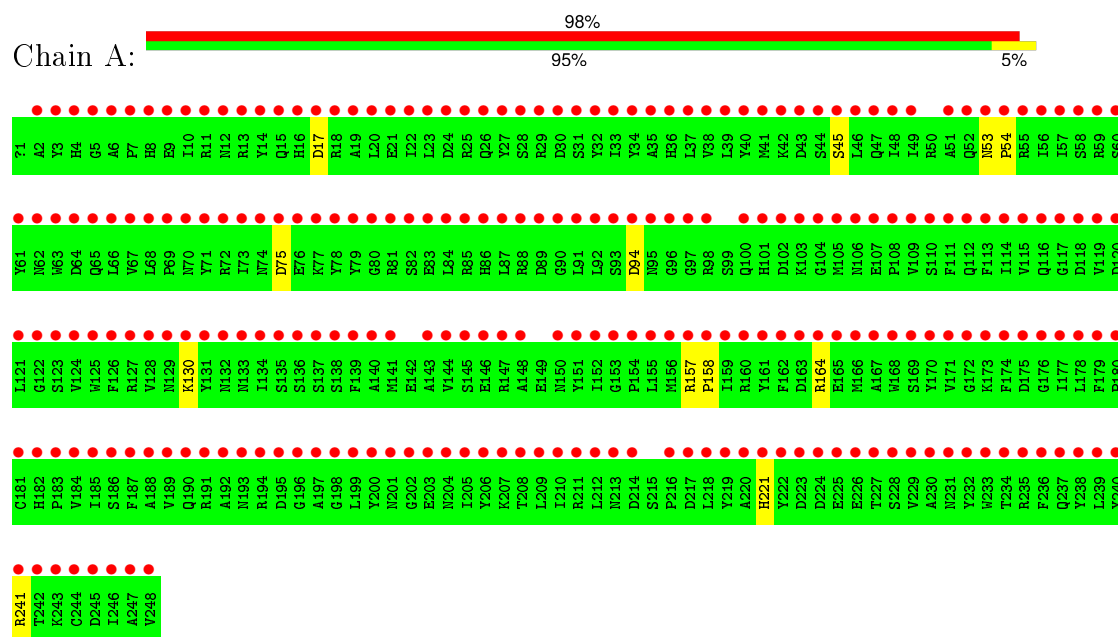
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	235	Total 235	O 235	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: POLYHEDRIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	102.72Å 102.72Å 102.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.94 – 1.51 51.36 – 1.51	Depositor EDS
% Data completeness (in resolution range)	74.0 (41.94-1.51) 74.0 (51.36-1.51)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.166 , 0.228 0.464 , 0.477	Depositor DCC
R_{free} test set	1045 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 507.4	EDS
Estimated twinning fraction	0.058 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 20980 reflections	Xtriage
F_o, F_c correlation	0.49	EDS
Total number of atoms	4301	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ATP, ACE

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	0.38	0/2110	0.53	0/2856

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	2058	1964	1959	7	2
2	A	31	12	12	0	1
3	A	1	0	0	0	0
4	A	235	0	0	3	1
All	All	2325	1976	1971	7	3

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 (7) 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:164:ARG:NH1	4:A:2040:HOH:O	2.15	0.79
1:A:164:ARG:NH1	4:A:2025:HOH:O	2.20	0.73
1:A:130:LYS:HD2	4:A:2154:HOH:O	2.06	0.56
1:A:45:SER:OG	1:A:221:HIS:HE1	1.96	0.48
1:A:75:ASP:OD2	1:A:221:HIS:HD2	1.97	0.48
1:A:53:ASN:CG	1:A:54:PRO:HD2	2.35	0.46
1:A:157:ARG:HA	1:A:158:PRO:HD3	1.86	0.43

All (3) 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:2042:HOH:O	4:A:2214:HOH:O[22_555]	1.70	0.50
1:A:241:ARG:HH12	2:A:1250:ATP:O1G[2_665]	1.55	0.05
1:A:17:ASP:OD2	1:A:17:ASP:OD2[4_565]	2.19	0.01

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	246/248 (99%)	236 (96%)	10 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	218/218 (100%)	217 (100%)	1 (0%)	92	81

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASP

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

Mol	Chain	Res	Type
1	A	221	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
2	ATP	A	1250	3	26,33,33	1.01	1 (3%)	26,52,52	1.74	3 (11%)

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	ATP	A	1250	3	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1250	ATP	C5-C4	3.19	1.47	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1250	ATP	N3-C2-N1	-7.05	123.33	128.87
2	A	1250	ATP	O3G-PG-O2G	2.23	115.62	107.44
2	A	1250	ATP	N6-C6-N1	2.49	122.70	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1250	ATP	0	1

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	247/248 (99%)	6.02	242 (97%) 0 0	9, 13, 22, 33	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	SER	16.5
1	A	3	TYR	15.6
1	A	63	TRP	15.4
1	A	109	VAL	14.4
1	A	40	TYR	14.1
1	A	134	ILE	13.7
1	A	33	ILE	13.6
1	A	66	LEU	13.0
1	A	139	PHE	12.8
1	A	227	THR	12.5
1	A	114	ILE	12.3
1	A	151	TYR	11.9
1	A	222	TYR	11.6
1	A	37	LEU	11.2
1	A	115	VAL	10.8
1	A	189	VAL	10.8
1	A	210	ILE	10.7
1	A	236	PHE	10.6
1	A	233	TRP	10.5
1	A	91	LEU	10.2
1	A	145	SER	10.0
1	A	198	GLY	10.0
1	A	49	ILE	10.0
1	A	206	TYR	10.0
1	A	51	ALA	10.0
1	A	178	LEU	9.9
1	A	125	TRP	9.8

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Mol	Chain	Res	Type	RSRZ
1	A	168	TRP	9.7
1	A	144	VAL	9.7
1	A	128	VAL	9.5
1	A	188	ALA	9.4
1	A	197	ALA	9.3
1	A	14	TYR	9.2
1	A	32	TYR	9.2
1	A	60	SER	9.2
1	A	5	GLY	8.6
1	A	205	ILE	8.5
1	A	170	TYR	8.4
1	A	34	TYR	8.4
1	A	84	LEU	8.3
1	A	219	TYR	8.3
1	A	119	VAL	8.3
1	A	155	LEU	8.3
1	A	238	TYR	8.2
1	A	45	SER	8.1
1	A	123	SER	8.1
1	A	10	ILE	8.1
1	A	229	VAL	8.0
1	A	232	TYR	8.0
1	A	29	ARG	7.9
1	A	216	PRO	7.9
1	A	161	TYR	7.8
1	A	160	ARG	7.8
1	A	87	LEU	7.7
1	A	164	ARG	7.6
1	A	74	ASN	7.6
1	A	194	ARG	7.6
1	A	234	THR	7.6
1	A	126	PHE	7.6
1	A	124	VAL	7.6
1	A	243	LYS	7.6
1	A	73	ILE	7.6
1	A	131	TYR	7.5
1	A	56	ILE	7.5
1	A	212	LEU	7.4
1	A	54	PRO	7.3
1	A	64	ASP	7.3
1	A	148	ALA	7.2
1	A	69	PRO	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	244	CYS	7.2
1	A	240	TYR	7.2
1	A	82	SER	7.1
1	A	28	SER	7.1
1	A	192	ALA	7.1
1	A	79	TYR	7.0
1	A	108	PRO	7.0
1	A	200	TYR	6.9
1	A	174	PHE	6.9
1	A	133	ASN	6.9
1	A	209	LEU	6.9
1	A	228	SER	6.8
1	A	46	LEU	6.8
1	A	106	ASN	6.7
1	A	248	VAL	6.7
1	A	171	VAL	6.7
1	A	111	PHE	6.7
1	A	140	ALA	6.7
1	A	16	HIS	6.6
1	A	158	PRO	6.6
1	A	62	ASN	6.5
1	A	166	MET	6.5
1	A	246	ILE	6.5
1	A	83	GLU	6.5
1	A	237	GLN	6.5
1	A	23	LEU	6.4
1	A	113	PHE	6.4
1	A	218	LEU	6.4
1	A	67	VAL	6.4
1	A	61	TYR	6.4
1	A	152	ILE	6.4
1	A	19	ALA	6.4
1	A	92	LEU	6.3
1	A	89	ASP	6.3
1	A	22	ILE	6.3
1	A	77	LYS	6.2
1	A	130	LYS	6.2
1	A	71	TYR	6.2
1	A	181	CYS	6.2
1	A	72	ARG	6.1
1	A	27	TYR	6.1
1	A	177	ILE	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	81	ARG	6.1
1	A	141	MET	6.0
1	A	110	SER	5.9
1	A	211	ARG	5.9
1	A	97	GLY	5.8
1	A	187	PHE	5.8
1	A	208	THR	5.8
1	A	154	PRO	5.7
1	A	157	ARG	5.6
1	A	47	GLN	5.6
1	A	183	PRO	5.6
1	A	86	HIS	5.6
1	A	35	ALA	5.6
1	A	103	LYS	5.5
1	A	38	VAL	5.5
1	A	36	HIS	5.5
1	A	57	ILE	5.5
1	A	159	ILE	5.5
1	A	68	LEU	5.5
1	A	100	GLN	5.4
1	A	31	SER	5.4
1	A	195	ASP	5.4
1	A	7	PRO	5.3
1	A	75	ASP	5.3
1	A	196	GLY	5.3
1	A	48	ILE	5.2
1	A	138	SER	5.2
1	A	121	LEU	5.2
1	A	6	ALA	5.2
1	A	204	ASN	5.1
1	A	180	PRO	5.1
1	A	143	ALA	5.0
1	A	163	ASP	5.0
1	A	135	SER	4.9
1	A	78	TYR	4.9
1	A	162	PHE	4.9
1	A	118	ASP	4.9
1	A	20	LEU	4.9
1	A	231	ASN	4.8
1	A	179	PHE	4.8
1	A	4	HIS	4.8
1	A	58	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	191	ARG	4.7
1	A	241	ARG	4.7
1	A	247	ALA	4.7
1	A	105	MET	4.7
1	A	85	ARG	4.7
1	A	176	GLY	4.6
1	A	39	LEU	4.6
1	A	12	ASN	4.6
1	A	175	ASP	4.5
1	A	184	VAL	4.5
1	A	53	ASN	4.4
1	A	9	GLU	4.4
1	A	136	SER	4.4
1	A	185	ILE	4.4
1	A	165	GLU	4.3
1	A	217	ASP	4.3
1	A	220	ALA	4.3
1	A	201	ASN	4.3
1	A	147	ARG	4.3
1	A	80	GLY	4.3
1	A	21	GLU	4.2
1	A	30	ASP	4.1
1	A	225	GLU	4.1
1	A	18	ARG	4.1
1	A	43	ASP	4.1
1	A	167	ALA	4.1
1	A	224	ASP	4.1
1	A	2	ALA	4.0
1	A	95	ASN	4.0
1	A	101	HIS	4.0
1	A	213	ASN	4.0
1	A	11	ARG	3.9
1	A	13	ARG	3.9
1	A	41	MET	3.9
1	A	129	ASN	3.9
1	A	59	ARG	3.8
1	A	117	GLY	3.8
1	A	156	MET	3.8
1	A	235	ARG	3.7
1	A	8	HIS	3.7
1	A	221	HIS	3.7
1	A	214	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	186	SER	3.6
1	A	96	GLY	3.5
1	A	132	ASN	3.5
1	A	25	ARG	3.5
1	A	17	ASP	3.5
1	A	199	LEU	3.5
1	A	65	GLN	3.4
1	A	153	GLY	3.4
1	A	182	HIS	3.4
1	A	104	GLY	3.3
1	A	137	SER	3.3
1	A	169	SER	3.3
1	A	242	THR	3.3
1	A	226	GLU	3.3
1	A	90	GLY	3.2
1	A	173	LYS	3.2
1	A	76	GLU	3.2
1	A	112	GLN	3.1
1	A	24	ASP	3.1
1	A	70	ASN	3.1
1	A	239	LEU	3.0
1	A	146	GLU	3.0
1	A	88	ARG	3.0
1	A	193	ASN	2.9
1	A	15	GLN	2.9
1	A	150	ASN	2.9
1	A	55	ARG	2.9
1	A	223	ASP	2.9
1	A	98	ARG	2.9
1	A	94	ASP	2.9
1	A	102	ASP	2.8
1	A	245	ASP	2.7
1	A	203	GLU	2.7
1	A	42	LYS	2.7
1	A	230	ALA	2.7
1	A	116	GLN	2.6
1	A	202	GLY	2.6
1	A	172	GLY	2.6
1	A	93	SER	2.5
1	A	52	GLN	2.4
1	A	190	GLN	2.3
1	A	26	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	122	GLY	2.2
1	A	207	LYS	2.2
1	A	120	ASP	2.1
1	A	107	GLU	2.1
1	A	127	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	MG	A	1251	1/1	0.87	0.65	5.50	17,17,17,17	0
2	ATP	A	1250	31/31	0.51	0.41	0.89	12,19,29,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.