



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5JD5 / pdb_00005jd5
Title : Crystal structure of MGS-MileE3, an alpha/beta hydrolase enzyme from the metagenome of pyrene-phenanthrene enrichment culture with sediment sample of Milazzo Harbor, Italy
Authors : Stogios, P.J.; Xu, X.; Cui, H.; Martinez-Martinez, M.; Chernikova, T.N.; Golyshin, P.N.; Yakimov, M.M.; Ferrer, M.; Savchenko, A.
Deposited on : 2016-04-15
Resolution : 1.95 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

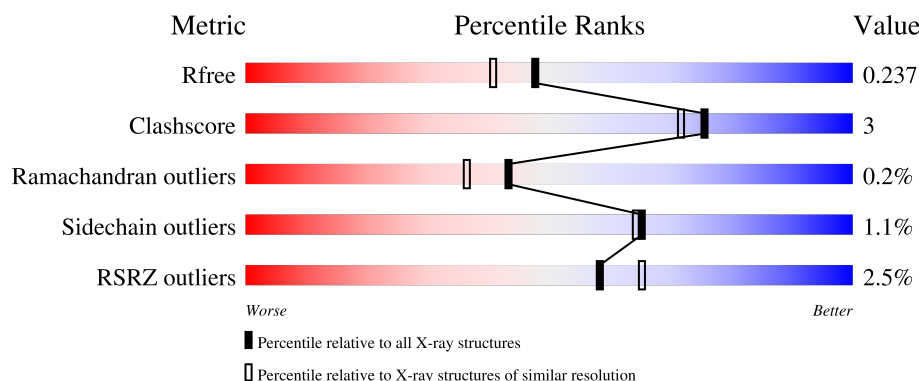
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	321	4% 90% 8% .
1	B	321	2% 92% 6% ..
1	C	321	2% 90% 7% ..
1	D	321	2% 90% 8% ..

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
1	OAS	A	169	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11745 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 MGS-Mile3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	2	0
			2435	1540	424	462	9			
1	B	318	Total	C	N	O	S	0	1	0
			2437	1540	424	464	9			
1	C	315	Total	C	N	O	S	0	2	0
			2417	1531	420	457	9			
1	D	317	Total	C	N	O	S	0	0	0
			2426	1534	423	460	9			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	536	Total	O	0	4
			540	540		
3	B	510	Total	O	0	3
			513	513		
3	C	481	Total	O	0	3
			484	484		
3	D	482	Total	O	0	9
			491	491		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.67Å 97.16Å 167.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.72 – 1.95 24.72 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.9 (24.72-1.95) 82.0 (24.72-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.195 , 0.237 0.196 , 0.237	Depositor DCC
R_{free} test set	2006 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11745	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 48.11 % 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 9.0183e-05. 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: OAS, CL

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	0.37	0/2494	0.73	1/3394 (0.0%)
1	B	0.35	1/2493 (0.0%)	0.70	0/3393
1	C	0.35	0/2476	0.74	1/3369 (0.0%)
1	D	0.34	0/2479	0.70	0/3374
All	All	0.35	1/9942 (0.0%)	0.72	2/13530 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	254	MET	C-O	-5.36	1.16	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	GLU	N-CA-C	12.09	126.47	112.93
1	A	54	GLU	N-CA-C	5.25	119.32	113.02

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	2435	0	2342	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2437	0	2338	13	0
1	C	2417	0	2332	15	0
1	D	2426	0	2329	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	540	0	0	2	0
3	B	513	0	0	4	0
3	C	484	0	0	3	1
3	D	491	0	0	2	1
All	All	11745	0	9341	57	1

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 3.

All (57) 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:169:OAS:HC22	3:A:816:HOH:O	1.87	0.72
1:C:148:LEU:HG	1:C:182:MET:HE1	1.73	0.70
1:C:235:GLU:OE1	1:C:235:GLU:N	2.25	0.69
1:A:169:OAS:HC23	1:A:295:HIS:NE2	2.14	0.63
1:B:52:ARG:NH1	3:B:504:HOH:O	2.33	0.61
1:B:50:ARG:NH1	3:B:501:HOH:O	2.35	0.58
1:A:184:ASP:OD2	1:D:34:THR:HG21	2.09	0.53
1:D:82:ILE:HD12	1:D:124:VAL:HG22	1.91	0.52
1:A:234:PRO:HB2	1:A:236:ASN:OD1	2.10	0.52
1:C:89:LYS:NZ	3:C:403:HOH:O	2.29	0.51
1:D:290:TYR:HB3	1:D:304:LEU:HD11	1.93	0.51
1:D:254:MET:HB3	1:D:278:TRP:CZ2	2.46	0.51
1:D:198:PHE:CZ	1:D:296:GLY:HA2	2.46	0.50
1:A:198:PHE:CZ	1:A:296:GLY:HA2	2.47	0.50
1:A:55:GLY:O	1:A:56:PRO:C	2.55	0.49
1:D:148:LEU:HG	1:D:182:MET:HE1	1.94	0.49
1:B:148:LEU:HG	1:B:182:MET:HE1	1.94	0.49
1:D:227:LYS:NZ	3:D:417:HOH:O	2.42	0.48
1:A:95:PHE:HE2	1:A:165:ILE:HD11	1.79	0.48
1:A:136:TYR:OH	1:A:243:ASP:OD2	2.31	0.47
1:A:216:ARG:NH2	1:A:264:ASP:OD2	2.46	0.47
1:C:300:PHE:HB2	3:C:541:HOH:O	2.14	0.47
1:B:169:OAS:HC23	1:B:295:HIS:NE2	2.29	0.47
1:C:111:MET:HG3	1:C:114:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:PHE:CZ	1:C:296:GLY:HA2	2.50	0.46
1:B:184:ASP:HB3	1:C:34[B]:THR:HG21	1.98	0.46
1:B:297:PHE:HA	1:B:300:PHE:CD2	2.51	0.46
1:D:234:PRO:O	1:D:237:VAL:HG22	2.15	0.46
1:C:155:LYS:HD3	1:C:161:ASP:OD2	2.17	0.45
1:D:235:GLU:CD	1:D:235:GLU:H	2.25	0.45
1:B:198:PHE:CZ	1:B:296:GLY:HA2	2.52	0.45
1:D:297:PHE:HA	1:D:300:PHE:CD2	2.52	0.44
1:B:4:ASP:OD1	1:B:5:ASN:N	2.50	0.44
1:C:318:ARG:NH1	3:C:419:HOH:O	2.50	0.44
1:B:234:PRO:HD2	1:B:237:VAL:HG11	1.99	0.44
1:A:169:OAS:OG	1:A:170:ALA:N	2.49	0.43
1:A:169:OAS:HC21	3:A:957:HOH:O	2.18	0.43
1:A:32:LEU:HB3	1:A:217:TYR:CD2	2.53	0.43
1:A:254:MET:HB3	1:A:278:TRP:CZ2	2.54	0.43
1:B:144:GLU:HG3	1:B:182:MET:CE	2.49	0.43
1:A:297:PHE:HA	1:A:300:PHE:CD2	2.54	0.43
1:B:254:MET:HB3	1:B:278:TRP:CZ2	2.54	0.43
1:D:95:PHE:HE2	1:D:165:ILE:HD11	1.84	0.42
1:C:254:MET:HB3	1:C:278:TRP:CZ2	2.54	0.42
1:C:82:ILE:HD12	1:C:124:VAL:HG22	2.01	0.42
1:D:229:ASP:OD1	1:D:239:ARG:NH2	2.52	0.42
1:D:290:TYR:HA	1:D:291:PRO:HD3	1.83	0.42
1:C:90:GLY:O	1:C:122:VAL:HG12	2.20	0.41
1:C:239:ARG:HG3	1:C:239:ARG:HH11	1.85	0.41
1:C:155:LYS:HD2	1:C:155:LYS:HA	1.83	0.41
1:A:197:VAL:HG12	1:A:198:PHE:CE1	2.56	0.41
1:B:155:LYS:NZ	3:B:533:HOH:O	2.54	0.41
1:C:95:PHE:HE2	1:C:165:ILE:HD11	1.86	0.41
1:A:32:LEU:HD11	1:A:219:ILE:HD13	2.02	0.40
1:B:7:PHE:HZ	3:B:624:HOH:O	2.04	0.40
1:D:321:ASP:OD2	3:D:401:HOH:O	2.22	0.40
1:A:236:ASN:OD1	1:A:237:VAL:HG13	2.21	0.40

All (1) 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)
3:C:853:HOH:O	3:D:834:HOH:O[1_545]	2.18	0.02

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	316/321 (98%)	309 (98%)	7 (2%)	0	100	100
1	B	316/321 (98%)	311 (98%)	4 (1%)	1 (0%)	36	28
1	C	314/321 (98%)	306 (98%)	7 (2%)	1 (0%)	36	28
1	D	314/321 (98%)	307 (98%)	6 (2%)	1 (0%)	36	28
All	All	1260/1284 (98%)	1233 (98%)	24 (2%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	198	PHE
1	D	198	PHE
1	B	198	PHE

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	246/247 (100%)	244 (99%)	2 (1%)	73	74
1	B	246/247 (100%)	244 (99%)	2 (1%)	73	74
1	C	244/247 (99%)	241 (99%)	3 (1%)	63	61
1	D	244/247 (99%)	240 (98%)	4 (2%)	55	52
All	All	980/988 (99%)	969 (99%)	11 (1%)	65	64

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

Mol	Chain	Res	Type
1	A	5	ASN
1	A	62	LYS
1	B	35	SER
1	B	122	VAL
1	C	44	GLU
1	C	223	LEU
1	C	235	GLU
1	D	122	VAL
1	D	162	LEU
1	D	223	LEU
1	D	235	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	153	ASN
1	D	25	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	OAS	A	169	1	7,8,9	1.24	1 (14%)	4,9,11	1.12	0
1	OAS	C	169	1	7,8,9	1.48	2 (28%)	4,9,11	2.76	1 (25%)
1	OAS	B	169	1	7,8,9	1.55	2 (28%)	4,9,11	1.54	1 (25%)
1	OAS	D	169	1	7,8,9	1.25	1 (14%)	4,9,11	1.43	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
1	OAS	A	169	1	-	2/5/7/9	-
1	OAS	C	169	1	-	0/5/7/9	-
1	OAS	B	169	1	-	2/5/7/9	-
1	OAS	D	169	1	-	2/5/7/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	OAS	OG-C1A	3.05	1.48	1.33
1	C	169	OAS	OG-C1A	2.89	1.47	1.33
1	A	169	OAS	OG-C1A	2.59	1.45	1.33
1	D	169	OAS	OG-C1A	2.33	1.44	1.33
1	B	169	OAS	CA-N	-2.23	1.41	1.48
1	C	169	OAS	OG-CB	-2.08	1.40	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	OAS	CB-OG-C1A	4.95	129.30	117.08
1	B	169	OAS	CB-OG-C1A	2.35	122.89	117.08

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	169	OAS	C2A-C1A-OG-CB
1	B	169	OAS	OAC-C1A-OG-CB
1	B	169	OAS	C2A-C1A-OG-CB
1	D	169	OAS	OAC-C1A-OG-CB
1	A	169	OAS	OAC-C1A-OG-CB
1	A	169	OAS	C2A-C1A-OG-CB

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	169	OAS	4	0
1	B	169	OAS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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	316/321 (98%)	-0.09	12 (3%) 44 50	16, 26, 62, 103	2 (0%)
1	B	317/321 (98%)	-0.15	5 (1%) 70 77	17, 25, 58, 93	1 (0%)
1	C	314/321 (97%)	-0.02	7 (2%) 62 69	15, 28, 54, 89	2 (0%)
1	D	316/321 (98%)	-0.04	8 (2%) 58 65	17, 27, 55, 108	0
All	All	1263/1284 (98%)	-0.08	32 (2%) 58 65	15, 27, 58, 108	5 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	PRO	4.3
1	D	320	THR	3.8
1	D	6	PRO	3.7
1	B	59	ALA	3.5
1	A	236	ASN	3.4
1	A	321	ASP	3.3
1	C	86	GLU	3.2
1	A	53	GLY	3.1
1	D	7	PHE	3.1
1	D	9	PRO	3.1
1	A	38	ASN	3.1
1	D	321	ASP	3.0
1	A	59	ALA	2.9
1	A	56	PRO	2.9
1	D	300	PHE	2.7
1	A	320	THR	2.7
1	A	50	ARG	2.7
1	D	236	ASN	2.5
1	C	10	GLU	2.5
1	A	51	ASP	2.4
1	B	51	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	5	ASN	2.3
1	C	7	PHE	2.2
1	C	236	ASN	2.2
1	A	86	GLU	2.2
1	A	237	VAL	2.2
1	B	30	ASP	2.2
1	B	50	ARG	2.2
1	C	300	PHE	2.1
1	C	8	ASP	2.1
1	A	57	PHE	2.0
1	B	86	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OAS	C	169	9/10	0.83	0.12	21,23,36,37	0
1	OAS	A	169	9/10	0.84	0.14	23,27,43,44	0
1	OAS	D	169	9/10	0.85	0.11	19,23,32,32	0
1	OAS	B	169	9/10	0.86	0.12	18,21,31,34	0

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(Å ²)	Q<0.9
2	CL	B	401	1/1	0.97	0.06	42,42,42,42	0
2	CL	A	401	1/1	0.98	0.04	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.